Chemical Information Review Document

for

Phenolic Benzotriazoles

Supporting Nomination for Toxicological Evaluation by the National Toxicology Program

October 2011

National Toxicology Program
National Institute of Environmental Health Sciences
National Institutes of Health
U.S. Department of Health and Human Services
Research Triangle Park, NC
http://ntp.niehs.nih.gov/

Abstract

Phenolic benzotriazoles are a class of ultraviolet-light absorbers. Compounds within this class are used in a variety of consumer applications including in polymers and sunscreens. Several of the phenolic benzotriazoles are produced by companies in China. Suppliers include those not only in China but also Belgium, Germany, and the United States. Production volumes for compounds within this class varied greatly according to 2006 Inventory Update Reporting records. The two main methods for the analysis of phenolic benzotriazoles are gas chromatography with mass spectrometry and high performance liquid chromatography. Combined with different sample preparation techniques, these can be applied to various media. Members of this chemical class have been detected in a variety of environmental samples including indoor dust, raw sewage, sewage treatment plant effluents, river water, river sediment, landfills, and marine sediment. Chemical levels were generally in the parts-per-billion to parts-per-trillion range within these samples. Human exposure may occur through oral or dermal exposure or through inhalation. Limited toxicological information was located for the chemicals within the class. Acute toxicity data were available for drometrizole, octrizole, ditBu-BZT, ditPe-BZT, diMeEtPh-BZT, bisoctrizole, and Tinuvin 1130 (reaction mixture product containing mPEG, dPEG, and polyethylene glycol). The oral LD_{50} values for chemicals with available data were ≥1000 mg/kg in mice and rats. Dermal LD_{50} values, obtained from four chemicals, were >2000 mg/kg in rats and >5000 mg/kg in rabbits. Inhalation LC_{50} values for drometrizole and octrizole in rats were >1420 mg/m^3 and >50 mg/L, respectively. Short-term and subchronic exposure studies were located for drometrizole, octrizole, ditBu-BZT, ditBu-ClBZT, ditPe-BZT, diMeEtPh-BZT, tBuPrAcid-BZT, tBuPrMeEst-BZT, tBuPrHexEst-BZT, and mPEG/dPEG (Tinuvin 1130). Overall, oral exposure to the tested chemicals led to liver effects in rats. Body weight and body weight gain changes and increased absolute and/or relative liver weights were observed. Histopathological changes and altered liver enzyme content and activities were noted after treatment with different phenolic benzotriazoles. Hematological effects were also observed. Chronic exposure studies were located for drometrizole and ditBu-BZT. Increased liver weights in absence of gross or microscopic changes were noted in mice, but not rats, after treatment with drometrizole for two years. Enlarged livers accompanied by histopathological changes were observed in rats treated with ditBu-BZT for 52 weeks. Hematological effects and increased relative organ weights were also observed after ditBu-BZT treatment at the highest dose. Drometrizole inhibited concanavalin A-stimulated rat spleen cell proliferation, and tBuPrAcid-BZT was cytotoxic to rat and guinea pig hepatocytes. Reproductive and teratological studies were located for drometrizole, ditBu-BZT, ditBu-ClBZT, ditPe-BZT, diMeEtPh-BZT, and mPEG/dPEG. Two of the tested compounds (i.e., drometrizole and ditBu-ClBZT) did not have any reproductive effects. While drometrizole did not affect pup development, ditBu-ClBZT exposure was shown to decrease pup body weight and increase liver weight. diMeEtPh-BZT exposure was associated with a non-dose-dependent decrease in fetal body weight and increase in skeletal maturation delay. Dam and fetal liver effects were noted after exposure to mPEG/dPEG. Additionally, muscular hemorrhages were observed. Reproductive and teratological effects after administration of Tinuvin 1130 suggested an association between dosing time and effect. Male and female MAGf (SPF) mice were fed ≤500 ppm drometrizole in diet daily for 24 months. Benign and malignant tumors were observed in both controls and treated mice but were not considered treatment related. Similarly, tumor formation in CFY male and female rats was not significantly different from controls and the distribution was not affected by treatment with ≤3000 ppm drometrizole for 104 weeks. None of the tested phenolic benzotriazoles were mutagenic *in vitro* in the absence or presence of a metabolic system or *in vivo*.

Executive Summary

Basis for Nomination

Phenolic benzotriazoles are a class of ultraviolet (UV)-light absorbers. Compounds within this class are used in a variety of consumer applications including in polymers and sunscreens. This class of chemicals was nominated by the National Institute of Environmental Health Sciences for toxicological testing based on its high production volume and widespread use. There is potential for exposure to workers and the general public. Additionally, the limited availability of toxicological data also contributes to the candidacy of these compounds for testing.

Nontoxicological Data

Several of the phenolic benzotriazoles are produced by companies in China. Suppliers include those not only in China but also Belgium, Germany, and the United States. Production volumes for compounds within this class varied greatly according to 2006 Inventory Update Reporting (IUR) records. While the aggregate production volumes of ditBu-ClBZT and bisoctrizole were <500,000 pounds, the production volumes of several other phenolic benzotrialzoles (e.g., octrizole) ranged between 1,000,000 and <10,000,000 pounds. The two main methods for the analysis of phenolic benzotriazoles are gas chromatography with mass spectrometry and high performance liquid chromatography. Combined with different sample preparation techniques, these can be applied to various media. The UV-light absorbing properties of these chemicals lend themselves for use in a variety of consumer products. Several chemicals (e.g., octrizole, drometrizole, and bumetrizole) are also used as fragrance ingredients. Chemicals within this class have been used in food packaging, candles, varnishes, cosmetics, and dental materials. One compound, octrizole, has also been used in an industrial pigment. Members of this chemical class have been detected in a variety of environmental samples including indoor dust, raw sewage, sewage treatment plant effluents, river water, river sediment, landfills, and marine sediment. Chemical levels were generally in the parts-per-billion to parts-per-trillion range within these samples. Human exposure to chemicals within this chemical class may occur through oral or dermal exposure or through inhalation. In addition to exposure through use of consumer products, oral exposure may occur through consumption of marine organisms containing these compounds. According to the 2006 IUR, the number of workers likely exposed to phenolic benzotriazoles from industrial manufacturing, processing, and use ranged from 1-99 to ≥1000. Several of the compounds within the class are regulated by the U.S. Environmental Protection Agency and the U.S. Food and Drug Administration.

Toxicological Data

A summary of the available toxicological data for phenolic benzotriazoles is provided in the table below. Studies on synergistic/antagonistic, initiation/promotion, cogenotoxicity, and immunotoxicity were not located for at least one of the chemicals within the class.

Chemical	CASRN	Human Data	Chemical Disposition, Metabolism, and Toxicokinetics	Acute Toxicity	Subchronic Toxicity	Chronic Toxicity	Cytotoxicity	Reproductive and Teratological Toxicity	Carcinogenicity	Genotoxicity	Other Data
Drometrizole	2440-22-4	X		X	X	X	X	X	X	X	X
Octrizole	3147-75-9	X		X	X					X	X
Bumetrizole	3896-11-5									X	X
ditBu-BZT	3846-71-7			X	X	X		X		X	
ditBu-ClBZT	3864-99-1				X			X		X	X

Chemical	CASRN	Human Data	Chemical Disposition, Metabolism, and Toxicokinetics	Acute Toxicity	Subchronic Toxicity	Chronic Toxicity	Cytotoxicity	Reproductive and Teratological Toxicity	Carcinogenicity	Genotoxicity	Other Data
ditPe-BZT	25973-55-1			X	X			X		X	X
diMeEtPh-BZT	70321-86-7			X	X			X		X	X
Bisoctrizole	103597-45-1	X		X							X
tBuPrAcid-BZT	84268-36-0		X		X		X				X
tBuPrMeEst-BZT	84268-33-7		X		X						
tBuPrHexEst-BZT	84268-08-6		X		X						
mPEG/dPEG (Tinuvin 1130)	104810-48-2/ 104810-47-1		X	X	X			X		X	X

Human Data

A repeat insult patch test with octrizole on volunteers was negative for skin sensitization. Drometrizole was proposed to induce contact allergy in 1 of 33 patients with suspected contact dermatitis. Six cases of allergic contact dermatitis was reported in individuals using Tinosorb® M (active ingredient: bisoctrizole) or a sunscreen containing the chemical.

Chemical Disposition, Metabolism, and Toxicokinetics

In vitro studies with tBuPrMeEst-BZT showed that it was hydrolyzed by rat serum, rat liver homogenates, and rat small intestine. Metabolism by rat small intestine homogenates was less efficient than liver metabolism. *In vitro m*etabolism of mPEG/dPEG was reduced compared to tBuPrMeEst-BZT using all three biological sources.

Male rats (n=2) were orally dosed with 10 mg/kg tBuPrMeEst-BZT or tBuPrHexEst-BZT. Maximal blood concentration of tBuPrMeEst-BZT (<2 μg_{pe}/g) was achieved under 2 hours. The apparent half-life was less than 12 hours. tBuPrAcid-BZT was the major metabolite formed. Compared to the high absorption of tBuPrMeEst-BZT, tBuPrHexEst-BZT absorption was lower (C_{max} was <0.13 μg_{pe}/g). The apparent half-life was ~12 hours. Hydrolysis played a major role in metabolism.

Acute Exposure

Acute toxicity data were available for drometrizole, octrizole, ditBu-BZT, ditPe-BZT, diMeEtPh-BZT, bisoctrizole, and Tinuvin 1130 (reaction mixture containing mPEG, dPEG, and polyethylene glycol). The oral LD_{50} values for chemicals with available data were ≥1000 mg/kg in mice and rats. Dermal LD_{50} values, obtained from four chemicals (octrizole, diMeEtPh-BZT, bisoctrizole, and Tinuvin 1130 [reaction mixture product containing mPEG, dPEG, and polyethylene glycol]), were >2000 mg/kg in rats and >5000 mg/kg in rabbits. Inhalation LC_{50} values for drometrizole and octrizole in rats were >1420 mg/m^3 and >50 mg/L, respectively.

Short-Term and Subchronic Exposure

Short-term and subchronic exposure studies were located for drometrizole, octrizole, ditBu-BZT, ditBu-ClBZT, ditPe-BZT, diMeEtPh-BZT, tBuPrAcid-BZT, tBuPrMeEst-BZT, tBuPrHexEst-BZT, and mPEG/dPEG (Tinuvin 1130). Overall, oral exposure of rats to the tested chemicals led to liver effects. Body weight and body weight gain changes and increased absolute and/or relative liver weights were observed in several studies. Histopathological changes (e.g., foci, hypertrophy, and cytoplasmic vacuolization) and altered liver enzyme content and activities were also noted after treatment with different phenolic benzotriazoles. Hematological effects (e.g., altered white and red blood cell counts, altered albumin levels, and packed cell volume) were observed. For those studies that calculated no observed adverse effect levels, the values ranged from <0.5 to ~5685 mg/kg/day.

Chronic Exposure

Chronic exposure studies were located for drometrizole and ditBu-BZT. Liver effects were noted in animals after treatment with both chemicals. Increased liver weights in absence of gross or microscopic changes were noted in mice after treatment with drometrizole for two years. A similar effect in rats treated with drometrizole was not noted. Enlarged livers accompanied by histopathological changes were observed in rats treated with ditBu-BZT for 52 weeks. Hematological effects and increased relative organ weights (e.g., brain and testes) were also observed after ditBu-BZT treatment at the highest dose.

Cytotoxicity

At a concentration of 13 µM, drometrizole inhibited concanavalin A-stimulated rat spleen cell proliferation by 6%. At concentrations >10 µM, tBuPrAcid-BZT was cytotoxic to rat and guinea pig hepatocytes.

Reproductive and Teratological Effects

Studies were located for drometrizole, ditBu-BZT, ditBu-ClBZT, ditPe-BZT, diMeEtPh-BZT, and mPEG/dPEG. Two of the tested compounds (i.e., drometrizole and ditBu-ClBZT) did not have any effects on reproduction indices (e.g., mating ratio or preimplantation loss). While drometrizole did not affect pup development, ditBu-ClBZT exposure was shown to decrease pup body weight and increase liver weight. diMeEtPh-BZT exposure was associated with a non-dose-dependent decrease in fetal body weight and increase in skeletal maturation delay. ditPe-BZT increased testes weights in male rats. Dam and fetal liver effects were noted after exposure to mPEG/dPEG. Additionally, muscular hemorrhages were observed. Some chemicals were shown to affect reproductive organ weights (e.g., ditBu-BZT). Studies with Tinuvin 1130 suggested an association between dosing time and effect. When dams were treated during gestation (days 6-15), minimal effects were noted. Comparatively, when rats were treated prior and during mating and during lactation, effects in reproductive parameters and pups were seen.

Carcinogenicity

Male and female MAGf (SPF) mice were fed ≤500 ppm drometrizole in diet daily for 24 months. Benign and malignant tumors were observed in both controls and treated mice but were not considered treatment related. Similarly, tumor formation in CFY male and female rats was not significantly different from controls, and the distribution was not affected by treatment with ≤3000 ppm drometrizole for 104 weeks.

Genotoxicity

Genotoxicity data were located for drometrizole, octrizole, bumetrizole, ditBu-BZT, ditBu-ClBZT, ditPe-BZT, diMeEtPh-BZT, and Tinuvin 1130. None of the tested compounds were identified as mutagenic *in vitro* in the absence or presence of a metabolic system or *in vivo*.

Other Data

Additional data were located for drometrizole, octrizole, bumetrizole, ditBu-ClBZT, ditPe-BZT, diMeEtPh-BZT, bisoctrizole, and Tinuvin 1130.

Structure-Activity Relationships

Structurally Similar Chemicals

Benzotriazole is the core structure present within the phenolic benzotriazole class. *In vitro* metabolism with rat liver microsomes yielded formation of 5- and 4-hydroxybenzotriazole (1.6 and 0.32% of the amount added, respectively); overall metabolism was low. Oral acute studies in rats and mice yielded LD_{50} values that ranged from 560 to 909 mg/kg. Intraperitoneal LD_{50} values in mice and rats ranged from

400-1000 and 500-900 mg/kg, respectively. A mouse intravenous LD_{50} of 238 mg/kg was identified. Dermal LD_{50} values were ≥1000 mg/kg in rats and rabbits and inhalation LC_{50} values in rats were 1.5 mg/L and 1.91 mg/L/3 hours. Subchronic and short-term studies showed that oral administration to mice produced minimal effects on body weight while dose-dependent decreases in body weight were observed in rats. Endocrine effects, normocytic anemia, and leukopenia were noted in rats dosed for 26 weeks. The TD_{Lo} was 109 mg/kg. No effects on deaths and no clinical symptoms were noted in mice or rats orally administered benzotriazole ≥78 weeks. Additionally, no dose-related effects on reproductive organs were noted in either sex. Neoplastic liver nodules were observed in male Fischer rats fed 12,100 ppm benzotriazole for 78 weeks. However, historic laboratory controls incidences varied from 0 to 11% so the treatment-related effects could not be determined. Brain tumors occurred in three males and one female rat. Incidence of endometrial stromal polyps was significant in female rats fed 6700 ppm for 78 weeks, but not in female rats fed 12,100 ppm. Significant increases in alveolar/bronchiolar carcinomas were observed in female B6C3F1 fed 11,700 ppm benzotriazole for 104 weeks. Comparatively, a similar increase was not observed in female mice fed 23,500 ppm benzotriazole for the same period of time. Genotoxicity studies indicate that the compound was not mutagenic to *Salmonella typhimurium* strains TA97, TA98, or TA100 in the presence or absence of S9, or Chinese hamster ovary cells. Benzotriazole was also not mutagenic to *S. typhimurium* strain TA1535 in the absence of S9, but was mutagenic in the presence of S9. Conflicting results were obtained for effects in *S. typhimurium* strains TA1537 and TA1538 and *Escherichia coli* WP2 *uvrA.* It did not produce DNA damage in *E. coli* PQ37. In Chinese hamster ovary cells, benzotriazole induced chromosomal aberrations in the presence of S9 and sister chromatid exchange in the absence of S9. Benzotriazole was not genotoxic in the mouse micronucleus assay at 800 mg/kg. Benzotriazole was identified as non-sensitizer in the guinea pig maximization test. Benzotriazole was identified as irritating to rabbit eyes and minimally irritating to rabbit and guinea pig skin.

<u>Leadscope</u>

For each Leadscope model suite evaluated, a positive prediction probability (ranging from 0-1) was calculated. Values >0.5 were defined as positive. If the test compound was not at least 30% similar to one in the training set and at least one model feature was not in the test compounds, the chemical was defined as "not in the domain" and prediction probability was not determined.

The models where seven or greater chemicals were predicted to be positive and discussed in the text were: SCE in vitro CHO and SCE in vitro Other Cells (genotoxicity), pup rodent behavior (neurotoxicity), structural rabbit (developmental), repo rat male (reproductive), repo rat female (reproductive), C3H10T1-2 (carcinogenicity), and palpitations (adverse human cardiological).

Genetic Toxicity

The 29 genetic toxicity models in Leadscope encompass predictions for mutagenicity (13), DNA damage (3), *in vivo* clastogenicity (5), and *in vitro* clastogenicity (8). The SCE in vitro CHO and SCE in vitro Other Cell models were the only models with ≥7 chemicals predicted to be positive. Prediction values for the SCE in vitro CHO model ranged from 0.522 to 0.88. Structural features in all chemicals identified as contributing negatively or positively to the predicted activity were aminobenzene, oxybenzene, benzene, and hydroxybenzene. The number of structurally similar chemicals for the positive compounds ranged from 1 to 14. Prediction values for the SCE in vitro Other Cells model ranged from 0.508 to 0.972. Structural features in all chemicals identified as contributing negatively or positively to the predicted activity were aminobenzene, oxybenzene, and benzene. The number of structurally similar chemicals for the positive compounds ranged from one to nine.

Neurotoxicity

The neurotoxicity models encompass predictions for newborn rat, rodent, and mouse behavior. The pup rodent behavior model was the only model with ≥7 chemicals predicted to be positive. Prediction values for the chemicals predicted to be positive ranged from 0.501 to 0.6355. Structural features in all chemicals identified as contributing negatively or positively to the predicted activity were oxybenzene and toluene. The number of structurally similar chemicals for the positive compounds ranged from one to four.

Reproductive and Developmental Toxicity

The developmental toxicity models encompass predictions for structural dysmorphogenesis, visceral organ toxicity, fetal survival, and fetal growth. The reproductive toxicity models encompass predictions for toxicity in male and female mice, rats, and rodents.

The structural rabbit model was the only developmental model with ≥7 chemicals predicted to be positive. Prediction values for the chemicals predicted to be positive ranged from 0.5227 to 0.769. Structural features in all chemicals identified as contributing negatively or positively to the predicted activity were 1-alkyl-4-hydroxybenzene, hydroxybenzene, 1-alkyl-2-hydroxybenzene, oxybenzene, 1,3-dialkylbenzene, 1,3-dimethylbenzene, toluene, benzene, ethylbenzene, and 1-(alkyl,acyc)-benzene. The number of structurally similar chemicals for the positive compounds ranged from two to seven.

The repo rat male and repo rat female models were the the reproductive models with ≥7 chemicals predicted to be positive. Prediction values for the chemicals predicted to be positive in the repo rat male model ranged from 0.537 to 0.745. Structural features in all chemicals identified as contributing negatively or positively to the predicted male reproduction activity were 1-alkyl-2-hydroxybenzene, oxybenzene, 1-(alkyl,acyc)-benzene, propane, and toluene. The number of structurally similar chemicals for the positive compounds ranged from one to two. Prediction values for the chemicals predicted to be positive in the repo rat female model ranged from 0.5092 to 0.792. A single structural feature in all chemicals was identified as contributing negatively or positively to the predicted female reproduction activity: benzene. The number of structurally similar chemicals for the positive compounds ranged from one to four.

Carcinogenicity

The chemicals were evaluated in two sets of carcinogenicity endpoint models; seven are rodent models based on the two-year rodent bioassays and four are cell transformation *in vitro* assay models. The C3H10T1-2 model was the only model with ≥7 chemicals predicted to be positive. Prediction values for the chemicals predicted to be positive ranged from 0.628 to 0.777. A single structural feature in all chemicals was identified as contributing negatively or positively to the predicted activity: propane. The number of structurally similar chemicals for the positive compounds was one.

Human Adverse Effects

Adverse cardiological, hepatobiliary, and urinary tract effects were evaluated in 24 models. The palpitations model was the only model with ≥7 chemicals predicted to be positive. Prediction values for the chemicals predicted to be positive ranged from 0.512 to 0.6875. Structural features in all chemicals identified as contributing negatively or positively to the predicted were t-butylbenzene, 1-(alkyl, acyc)-benzene, toluene, oxybenzene, and hydroxybenzene. The number of structurally similar chemicals for the positive compounds ranged from 1 to 13.

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Chemical Information Review Document for Phenolic Benzotriazoles

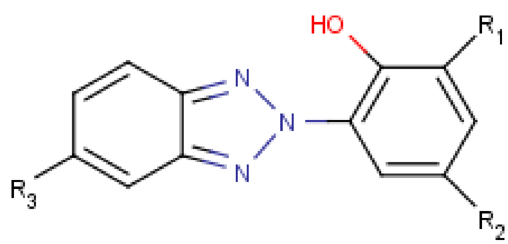
Tables:

1.0 Basis for Nomination

Phenolic benzotriazoles are a class of ultraviolet (UV)-light absorbers. Compounds within this class are used in a variety of consumer applications including in polymers and sunscreens. This class of chemicals was nominated by the National Institute of Environmental Health Sciences for toxicological testing based on its high production volume and widespread use. There is potential for exposure to workers and the general public. Additionally, the limited availability of toxicological data also contributes to the candidacy of these compounds for testing.

2.0 Introduction

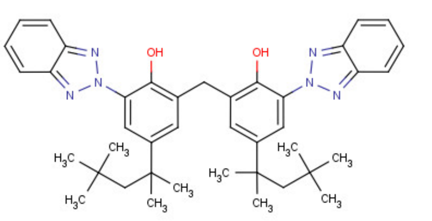
The following compounds were used to define the phenolic benzotriazole chemical class. Overall, the chemicals contain a benzotriazole central moiety with a 2-phenol attached at the 2-position. Substituents on the phenol were generally located at the 3- and 5-positions. The generic structure and following table provide details on chemical name, Chemical Abstracts Service Registry Number (CASRN), and substituent location. The abbreviations used in this report for each chemical are also provided in the following table.



Chemical Name	Name Used in Report	CASRN	R_1	R_2	R_3
2-(2H-Benzotriazol-2-yl)phenol	P-BZT	10096-91-0	H	H	H
Drometrizole	Drometrizole	2440-22-4	H	CH_3	H
2-(2H-Benzotriazol-2-yl)-4-(1,1-dimethylethyl)phenol	tBu-BZT	3147-76-0	H	$C(CH_3)_3$	H
2-(5-Chloro-2H-benzotriazol-2-yl)-4-(1,1-dimethylethyl)phenol	tBu-ClBZT	3287-17-0	H	$C(CH_3)_3$	Cl
Octrizole	Octrizole	3147-75-9	H	$C(CH_3)_2CH_2C(CH_3)_3$	H
3-(2H-Benzotriazol-2-yl)-4-hydroxybenzeneethanol	EtOH-BZT	96549-95-0	H	CH_2CH_2OH	H
1-[3-(2H-Benzotriazol-2-yl)-4-hydroxyphenyl]ethanone	Ethanone-BZT	83741-30-4	H	$COCH_3$	H
4-(2-Methacryloyloxyethyl)-2-(2H-benzotriazol-2-yl)phenol	MaOE-BZT	96478-09-0	H	$(CH_2)_2OC(O)CH(CH_2)(CH_3)$	H
2-(2H-Benzotriazol-2-yl)-4-methyl-6-(2-propenyl)phenol	Allyl-BZT	2170-39-0	CH_2CHCH_2	CH_3	H
2-(2H-Benzotriazol-2-yl)-6-dodecyl-4-methylphenol	DoM-BZT	23328-53-2	$(CH_2)_{11}CH_3$	CH_3	H
2-(2H-Benzotriazol-2-yl)-4-(1,1-dimethylethyl)-6-(1-methylpropyl)phenol	sButBu-BZT	36437-37-3	$CH_3CHCH_2CH_3$	$C(CH_3)_3$	H
Bumetrizole	Bumetrizole	3896-11-5	$C(CH_3)_3$	CH_3	Cl
2-(2H-Benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)phenol	ditBu-BZT	3846-71-7	$C(CH_3)_3$	$C(CH_3)_3$	H
2-(5-Chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)phenol	ditBu-ClBZT	3864-99-1	$C(CH_3)_3$	$C(CH_3)_3$	Cl

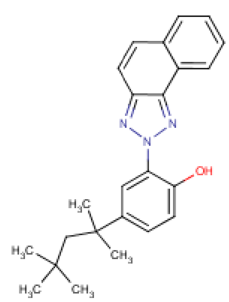
Chemical Name	Name Used in Report	CASRN	R_1	R_2	R_3
2-(2H-Benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)phenol	ditPe-BZT	25973-55-1	$C(CH_3)_2CH_2CH_3$	$C(CH_3)_2CH_2CH_3$	H
2-(2H-Benzotriazol-2-yl)-4,6-bis(1,1,3,3-tetramethylbutyl)phenol	ditOc-BZT	70693-49-1	$C(CH_3)_2CH_2C(CH_3)_3$	$C(CH_3)_2CH_2C(CH_3)_3$	H
2-(2H-Benzotriazol-2-yl)-6-(1-methyl-1-phenylethyl)-4-(1,1,3,3-tetramethylbutyl)phenol	MeEtPhMeBu-BZT	73936-91-1	$C(CH_3)_2(C_6H_5)$	$C(CH_3)_2CH_2C(CH_3)_3$	H
2-(1-Methyl-1-phenylethyl)-4-(1,1,3,3-tetramethylbutyl)-6-[5-(trifluoromethyl)-2H-benzotriazol-2-yl]phenol	MeEtMeBu-CF_3BZT	207738-63-4	$C(CH_3)_2(C_6H_5)$	$C(CH_3)_2CH_2C(CH_3)_3$	CF_3
2-(2H-Benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol	diMeEtPh-BZT	70321-86-7	$C(CH_3)_2(C_6H_5)$	$C(CH_3)_2(C_6H_5)$	H
3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid	tBuPrAcid-BZT	84268-36-0	$C(CH_3)_3$	$(CH_2)_2COOH$	H
3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, methyl ester	tBuPrMeEst-BZT	84268-33-7	$C(CH_3)_3$	$CH_2CH_2COOCH_3$	H
3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, 1,6-hexanediyl ester	tBuPrHexEst-BZT	84268-08-6	$C(CH_3)_3$	$(CH_2)_2COO(CH_2)_5CH_3$	H
3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, octyl ester	tBuPrOcEst-BZT	84268-23-5	$C(CH_3)_3$	$(CH_2)_2COO(CH_2)_7CH_3$	H
3-(5-Chloro-2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, octyl ester	tBuPrOcEst-ClBZT	83044-89-7	$C(CH_3)_3$	$(CH_2)_2COO(CH_2)_7CH_3$	Cl
3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-benzenepropanoic acid, C_{7-9}-branched and linear alkyl esters	tBu(C_{7-9})Est-BZT	127519-17-9	$C(CH_3)_3$	$(CH_2)_2COO(CH_2)_3CH(CH_3)CH_2H_3$	H

In addition to the chemicals noted above, the following chemicals were included in this class:



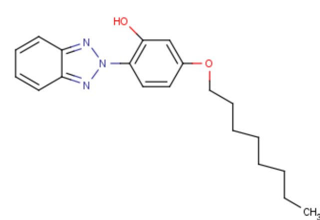
Bisoctrizole

Name Used in Report: Bisoctrizole
103597-45-1



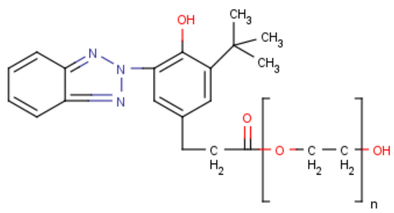
2-(2H-Naphtho(1,2-*d*)triazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol

Name Used in Report: Oc-NTZ
27876-55-7



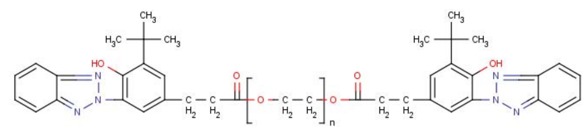
2-(2H-Benzotriazol-2-yl)-5-(octyloxy)phenol

Name Used in Report: OcOx-BZT
3147-77-1



Polyethylene glycol mono-3-(3-(2H-benzotriazol-2-yl)-5-*tert*-butyl-4-hydroxyphenyl)-1-oxopropyl ether

Name Used in Report: mPEG
104810-48-2†



Polyethylene glycol di(3-(3-(2H-benzotriazol-2-yl)-5-*tert*-butyl-4-hydroxyphenyl)-1-oxopropyl) ether

Name Used in Report: dPEG
104810-47-1‡

†According to Registry, this CASRN is associated with the trade name Tinuvin 1130. In contrast, ChemIDplus associates the trade name with CASRN 84268-33-7 (i.e., BZT-Pr acid, ME). ‡Internet searches show that the trade name Tinuvin 1130 is also associated with CASRN 104810-47-1 or with both (i.e., 104810-47-1 and 104810-48-2] (e.g., chemBlink, 2011; Chemical Book, 2008a; and ChemNet, undated). [Note: Another source lists the trade name Tinuvin 213 for CASRN 104810-48-2 and Tinuvin-1130 with CASRN 104810-47-1. See **Table 1**.]

2.1 Chemical Identification and Analysis

The phenolic benzotriazoles reviewed in this report are described in **Table 1**. Only a few synonyms are noted here; additional names are provided in Appendix C.

Table 1. Chemical Identification of Evaluated Phenolic Benzotriazoles

Chemical Name	Formula	Mol. Wt.	Synonyms	PubChem CID	InChI	Canonical SMILES
P-BZT	$C_{12}H_9N_3O$	211.22	2-(2-Hydroxyphenyl)benzotriazole	N/A	N/A	N/A
Drometrizole	$C_{13}H_{11}N_3O$	225.25	2-(5-Methyl-2-hydroxyphenyl)benzotriazole 2-Benzotriazol-2-yl-4-methylphenol Eversorb 71 Tinuvin P	17113	InChI=1S/C13H11N3O/c1-9-6-7-13(17)12(8-9)16-14-10-4-2-3-5-11(10)15-16/h2-8,17H,1H3	CC1=CC(=C(C=C1)O)N2N=C3C=CC=CC3=N2
tBu-BZT	$C_{16}H_{17}N_3O$	267.33	2-(2-Hydroxy-5-*tert*-butyl)benzotriazole 2-(5-*tert*-Butyl-2-hydroxyphenyl)benzotriazole Eversorb 70 Tinuvin PS	76605	InChI=1S/C16H17N3O/c1-16(2,3)11-8-9-15(20)14(10-11)19-17-12-6-4-5-7-13(12)18-19/h4-10,20H,1-3H3	CC(C)(C)C1=CC(=C(C=C1)O)N2N=C3C=CC=CC3=N2
tBu-ClBZT	$C_{16}H_{16}ClN_3O$	301.77	2-(2'-Hydroxy-5'-*tert*-butylphenyl)-5-chlorobenzotriazole Tinuvin 301	3014188	InChI=1S/C16H16ClN3O/c1-16(2,3)10-4-7-15(21)14(8-10)20-18-12-6-5-11(17)9-13(12)19-20/h4-9,21H,1-3H3	CC(C)(C)C1=CC(=C(C=C1)O)N2N=C3C=CC(=CC3=N2)Cl
Octrizole	$C_{20}H_{25}N_3O$	323.43	2-(2'-Hydroxy-5'-*tert*-octylphenyl)benzotriazole Eversorb 72 Tinuvin 329	62485	InChI=1S/C20H25N3O/c1-19(2,3)13-20(4,5)14-10-11-18(24)17(12-14)23-21-15-8-6-7-9-16(15)22-23/h6-12,24H,13H2,1-5H3	CC(C)(C)CC(C)(C)C1=CC(=C(C=C1)O)N2N=C3C=CC=CC3=N2
EtOH-BZT	$C_{14}H_{13}N_3O_2$	255.27	2-(2'-Hydroxy-5'-(2-hydroxyethyl)phenyl)benzotriazole	688251	InChI=1S/C14H13N3O2/c18-8-7-10-5-6-14(19)13(9-10)17-15-11-3-1-2-4-12(11)16-17/h1-6,9,18-19H,7-8H2	C1=CC2=NN(N=C2C=C1)C3=C(C=CC(=C3)CCO)O
Ethanone-BZT	$C_{14}H_{11}N_3O_2$	253.26	[*none provided*]	158568	InChI=1S/C14H11N3O2/c1-9(18)10-6-7-14(19)13(8-10)17-15-11-4-2-3-5-12(11)16-17/h2-8,19H,1H3	CC(=O)C1=CC(=C(C=C1)O)N2N=C3C=CC=CC3=N2
MaOE-BZT	$C_{18}H_{17}N_3O_3$	323.35	2-(2'-Hydroxy-5'-(2-methacryloyloxyethyl)phenyl)benzotriazole 2-[3-(2H-Benzotriazol-2-yl)-4-hydroxyphenyl]ethyl methacrylate	N/A	InChI=1S/C18H17N3O3/c1-12(2)18(23)24-10-9-13-7-8-17(22)16(11-13)21-19-14-5-3-4-6-15(14)20-21/h3-8,11,22H,1,9-10H2,2H3 [*ChemIDplus*]	n1(nc2c(n1)cccc2)c1c(ccc(c1)CCOC(=O)C(=C)C)O [not canonical; *ChemIDplus*]
Allyl-BZT	$C_{16}H_{15}N_3O$	265.31	2-(3'-Allyl-2'-hydroxy-5'-methylphenyl)benzotriazole 2-Allyl-6-(2H-benzotriazol-2-yl)p-cresol	N/A	N/A	N/A
DoM-BZT	$C_{25}H_{35}N_3O$	393.56	(2-Hydroxy-3-dodecyl-5-methylphenyl)benzotriazole 2-(3-Dodecyl-2-hydroxy-5-methylphenyl)benzotriazole Tinuvin 171 Tinuvin 571	86375	InChI=1S/C25H35N3O/c1-3-4-5-6-7-8-9-10-11-12-15-21-18-20(2)19-24(25(21)29)28-26-22-16-13-14-17-23(22)27-28/h13-14,16-19,29H,3-12,15H2,1-2H3	CCCCCCCCCCCCC1=C(C(=CC(=C1)C)N2N=C3C=CC=CC3=N2)O
sButBu-BZT	$C_{20}H_{25}N_3O$	323.43	2-(2-Hydroxy-3-*sec*-butyl-5-*tert*-butylphenyl) benzotriazole 2-(3-*sec*-Butyl-5-*tert*-butyl-2-hydroxyphenyl)benzotriazole Eversorb 79 Tinuvin 350†	118327	InChI=1S/C20H25N3O/c1-6-13(2)15-11-14(20(3,4)5)12-18(19(15)24)23-21-16-9-7-8-10-17(16)22-23/h7-13,24H,6H2,1-5H3	CCC(C)C1=C(C(=CC(=C1)C(C)(C)C)N2N=C3C=CC=CC3=N2)O
Bumetrizole	$C_{17}H_{18}ClN_3O$	315.80	2-(2'-Hydroxy-3'-*tert*-butyl-5'-methylphenyl)-5-chlorobenzotriazole Eversorb 73 Tinuvin [*ChemIDplus*] Tinuvin 326	62531	InChI=1S/C17H18ClN3O/c1-10-7-12(17(2,3)4)16(22)15(8-10)21-19-13-6-5-11(18)9-14(13)20-21/h5-9,22H,1-4H3	CC1=CC(=C(C(=C1)N2N=C3C=CC(=CC3=N2)Cl)O)C(C)(C)C

Chemical Name	Formula	Mol. Wt.	Synonyms	PubChem CID	InChI	Canonical SMILES
ditBu-BZT	$C_{20}H_{25}N_3O$	323.43	2-(2-Hydroxy-3,5-di-*tert*-butylphenyl)benzotriazole 2-Benzotriazol-2-yl-4,6-di-*tert*-butylphenol [*ChemIDplus*] Eversorb 77 Tinuvin 320	77455	InChI=1S/C20H25N3O/c1-19(2,3)13-11-14(20(4,5)6)18(24)17(12-13)23-21-15-9-7-8-10-16(15)22-23/h7-12,24H,1-6H3	CC(C)(C)C1=CC(=C(C(=C1)N2N=C3C=CC=CC3=N2)O)C(C)(C)C
ditBu-ClBZT	$C_{20}H_{24}ClN_3O$	357.88	2-(3,5-Di-*tert*-butyl-2-hydroxyphenyl)-5-chlorobenzotriazole 5-Chloro-2-(2-hydroxy-3,5-di-*tert*-butylphenyl)benzotriazole Eversorb 75 Tinuvin 327	77470	InChI=1S/C20H24ClN3O/c1-19(2,3)12-9-14(20(4,5)6)18(25)17(10-12)24-22-15-8-7-13(21)11-16(15)23-24/h7-11,25H,1-6H3	CC(C)(C)C1=CC(=C(C(=C1)N2N=C3C=CC(=CC3=N2)Cl)O)C(C)(C)C
ditPe-BZT	$C_{22}H_{29}N_3O$	351.49	2-(2-Hydroxy-3,5-di-*tert*-pentylphenyl)benzotriazole 2-(3,5-Di-*tert*-pentyl-2-hydroxyphenyl)benzotriazole Eversorb 74 Tinuvin 328	33263	InChI=1S/C22H29N3O/c1-7-21(3,4)15-13-16(22(5,6)8-2)20(26)19(14-15)25-23-17-11-9-10-12-18(17)24-25/h9-14,26H,7-8H2,1-6H3	CCC(C)(C)C1=CC(=C(C(=C1)N2N=C3C=CC=CC3=N2)O)C(C)(C)CC
ditOc-BZT	$C_{28}H_{41}N_3O$	435.64	2-(Benzotriazol-2-yl)-4,6-bis(2,4,4-trimethylpentan-2-yl)phenol [*PubChem*] 2-(2-Hydroxy-3,5-bis(*tert*-octyl)phenyl)benzotriazole [*ChemIDplus*]	116809	InChI=1S/C28H41N3O/c1-25(2,3)17-27(7,8)19-15-20(28(9,10)18-26(4,5)6)24(32)23(16-19)31-29-21-13-11-12-14-22(21)30-31/h11-16,32H,17-18H2,1-10H3	CC(C)(C)CC(C)(C)C1=CC(=C(C(=C1)N2N=C3C=CC=CC3=N2)O)C(C)(C)CC(C)(C)C
MeEtPhMeBu-BZT	$C_{29}H_{35}N_3O$	441.61	2-[2'-Hydroxy-3'-(α,α-dimethylbenzyl)-5'-(1,1,3,3-tetramethylbutyl)phenyl]benzotriazole Tinuvin 928	9803353	InChI=1S/C29H35N3O/c1-27(2,3)19-28(4,5)21-17-22(29(6,7)20-13-9-8-10-14-20)26(33)25(18-21)32-30-23-15-11-12-16-24(23)31-32/h8-18,33H,19H2,1-7H3	CC(C)(C)CC(C)(C)C1=CC(=C(C(=C1)N2N=C3C=CC=CC3=N2)O)C(C)(C)C4=CC=CC=C4
MeEtMeBu-CF_3BZT	$C_{30}H_{34}F_3N_3O$	509.61	5-Trifluoromethyl-2-[2-hydroxy-3-α-cumyl-5-*tert*-octylphenyl]-2H-benzotriazole	N/A	InChI=1S/C30H34F3N3O/c1-27(2,3)18-28(4,5)21-15-22(29(6,7)19-11-9-8-10-12-19)26(37)25(17-21)36-34-23-14-13-20(30(31,32)33)16-24(23)35-36/h8-17,37H,18H2,1-7H3 [*ChemSpider*]	FC(F)(F)c1ccc2nn(nc2c1)c3cc(cc(c3O)C(c4ccccc4)(C)C)C(C)(C)CC(C)(C)C [not canonical; *ChemSpider*]
diMeEtPh-BZT	$C_{30}H_{29}N_3O$	447.57	2-[2-Hydroxy-3,5-bis(α,α-dimethylbenzyl)phenyl]benzotriazole Eversorb 234 Eversorb 76 Tinuvin 234 Tinuvin 234D Tinuvin 900	112412	InChI=1S/C30H29N3O/c1-29(2,21-13-7-5-8-14-21)23-19-24(30(3,4)22-15-9-6-10-16-22)28(34)27(20-23)33-31-25-17-11-12-18-26(25)32-33/h5-20,34H,1-4H3	CC(C)(C1=CC=CC=C1)C2=CC(=C(C(=C2)N3N=C4C=CC=CC4=N3)O)C(C)(C)C5=CC=CC=C5
tBuPrAcid-BZT	$C_{19}H_{21}N_3O_3$	339.39	3-[3-(2H-Benzotriazol-2-yl)-5-*tert*-butyl-4-hydroxyphenyl]propionic acid	158619	InChI=1S/C19H21N3O3/c1-19(2,3)13-10-12(8-9-17(23)24)11-16(18(13)25)22-20-14-6-4-5-7-15(14)21-22/h4-7,10-11,25H,8-9H2,1-3H3,(H,23,24)	CC(C)(C)C1=C(C(=CC(=C1)CCC(=O)O)N2N=C3C=CC=CC3=N2)O
tBuPrMeEst-BZT	$C_{20}H_{23}N_3O_3$	353.41	2-[3'-*tert*-Butyl-2'-hydroxy-5'-(2-methoxycarbonylethyl)phenyl]benzotriazole Tinuvin 1130 [*ChemIDplus*][a]	93481	InChI=1S/C20H23N3O3/c1-20(2,3)14-11-13(9-10-18(24)26-4)12-17(19(14)25)23-21-15-7-5-6-8-16(15)22-23/h5-8,11-12,25H,9-10H2,1-4H3	CC(C)(C)C1=C(C(=CC(=C1)CCC(=O)OC)N2N=C3C=CC=CC3=N2)O
tBuPrHexEst-BZT	$C_{25}H_{33}N_3O_3$[b]	423.55	1,6-Hexanediyl bis(3-benzotriazol-2-yl)-4-hydroxy-5-*tert*-butyl)phenylpropionate Tinuvin 840	3086183	InChI=1S/C25H33N3O3/c1-5-6-7-10-15-31-23(29)14-13-18-16-19(25(2,3)4)24(30)22(17-18)28-26-20-11-8-9-12-21(20)27-28/h8-9,11-12,16-17,30H,5-7,10,13-15H2,1-4H3	CCCCCCOC(=O)CCC1=CC(=C(C(=C1)N2N=C3C=CC=CC3=N2)O)C(C)(C)C

Chemical Name	Formula	Mol. Wt.	Synonyms	PubChem CID	InChI	Canonical SMILES
tBuPrOcEst-BZT	$C_{27}H_{37}N_3O_3$	451.60	2-[3'-*tert*-Butyl-2'-hydroxy-5'-(2-octyloxycarbonylethyl)phenyl]benzotriazole Tinuvin 384 Tinuvin 99 Tinuvin 99/2	N/A	N/A	N/A
tBuPrOcEst-ClBZT	$C_{27}H_{36}ClN_3O_3$	486.05	2-(3'-*tert*-Butyl-5'-(2-octyloxycarbonylethyl)-2'-hydroxyphenyl)-5-chlorobenzotriazole	174297	InChI=1S/C27H36ClN3O3/c1-5-6-7-8-9-10-15-34-25(32)14-11-19-16-21(27(2,3)4)26(33)24(17-19)31-29-22-13-12-20(28)18-23(22)30-31/h12-13,16-18,33H,5-11,14-15H2,1-4H3	CCCCCCCCOC(=O)CCC1=CC(=C(C(=C1)N2N=C3C=CC(=CC3=N2)Cl)O)C(C)(C)C
tBu(C_{7-9})Est-BZT	$C_{26}H_{35}N_3O_3$[c]	437.57	4-Methylhexyl 3-[3-(benzotriazol-2-yl)-5-*tert*-butyl-4-hydroxyphenyl]propanoate [*PubChem*] Tinuvin 384‡	86220	InChI=1S/C26H35N3O3/c1-6-18(2)10-9-15-32-24(30)14-13-19-16-20(26(3,4)5)25(31)23(17-19)29-27-21-11-7-8-12-22(21)28-29/h7-8,11-12,16-18,31H,6,9-10,13-15H2,1-5H3	CCC(C)CCCOC(=O)CCC1=CC(=C(C(=C1)N2N=C3C=CC=CC3=N2)O)C(C)(C)C
Bisoctrizole	$C_{41}H_{50}N_6O_2$	658.87	2,2'-Methylenebis[6-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol] Eversorb 78 Tinuvin 360	3571576	InChI=1S/C41H50N6O2/c1-38(2,3)24-40(7,8)28-20-26(36(48)34(22-28)46-42-30-15-11-12-16-31(30)43-46)19-27-21-29(41(9,10)25-39(4,5)6)23-35(37(27)49)47-44-32-17-13-14-18-33(32)45-47/h11-18,20-23,48-49H,19,24-25H2,1-10H3	CC(C)(C)CC(C)(C)C1=CC(=C(C(=C1)N2N=C3C=CC=CC3=N2)O)CC4=C(C(=CC(=C4)C(C)(C)CC(C)(C)C)N5N=C6C=CC=CC6=N5)O
Oc-NTZ	$C_{24}H_{27}N_3O$	373.49	2-(2'-Hydroxy-5'-t-octylphenyl)naphthotriazole	119736	InChI=1S/C24H27N3O/c1-23(2,3)15-24(4,5)17-11-13-21(28)20(14-17)27-25-19-12-10-16-8-6-7-9-18(16)22(19)26-27/h6-14,28H,15H2,1-5H3	CC(C)(C)CC(C)(C)C1=CC(=C(C=C1)O)N2N=C3C=CC4=CC=CC=C4C3=N2
OcOx-BZT	$C_{20}H_{25}N_3O_2$	339.43	2-(2'-Hydroxy-4'-octyloxyphenyl)benzotriazole	N/A	N/A	N/A
mPEG	$(C_2H_4O)_nC_{19}H_{21}N_3O_3$	N/A	α-[3-[3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropyl]-Ω-hydroxypoly(oxy-1,2-ethanediyl) Tinuvin 1130[a,d]	N/A	N/A	N/A
dPEG	$(C_2H_4O)_nC_{38}H_{40}N_6O_5$	N/A	α-[3-[3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropyl]-Ω-[3-[3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy]poly(oxy-1,2-ethanediyl)	N/A	N/A	N/A

Sources: PubChem (undated-a); Registry (2010, 2011) [Note: When no synonyms were provided in the Registry record, any available from the ChemIDplus, PubChem, and/or ChemSpider record(s) was(were) reported.]
†Chemical Book (2008b); Tetrahedron (2010)
‡Chemical Book (2008c); NICNAS (1993)
[a]According to Registry, CASRN 104810-48-2is associated with the trade name Tinuvin 1130. In contrast, ChemIDplus associates the trade name with CASRN 84268-33-7. [Internet searches show that the trade name is also associated with CASRN 104810-47-1 or with both (i.e., 104810-47-1 and 104810-48-2] (e.g., chemBlink, 2011; Chemical Book, 2008a; and ChemNet, undated).]
[b]According to Registry, the formula is $C_{44}H_{52}N_6O_6$ with molecular weight of 760.92.
[c]According to Registry and ChemIDplus, the formula is unspecified.
[d]According to BuyersGuideChem, the trade name for this CASRN is Tinuvin 213. "1130" is only associated with the name UV-1130 (BuyersGuideChem, 2011r). [Note: UN-1130, however, is also listed as a synonym for CASRN 104810-47-1. In addition, the tradename Tinuvin-1130 is associated with this latter CASRN (BuyersGuideChem, 2011s).]

Chemical Analysis

The two main methods for the analysis of phenolic benzotriazoles are gas chromatography with mass spectrometry (GC-MS) and high performance liquid chromatography (HPLC). Combined with different sample preparation techniques, these can be applied to various media. Examples are provided below.

UV stabilizers in polyethylene terephthalate (PET) bottles can be determined using GC-MS. The high specificity, quantitative precision, and accuracy allow further application in migration studies. For octrizole, the detection limit was 19 pg and the mean recovery rate from extraction was 83.4% (Monteiro et al., 1998). Another method for the analysis of UV stabilizers in PET bottles is size exclusion chromatography-HPLC. The detection limit for octrizole was 0.1 µg/kg, and the mean recovery rate from extraction was 69.3% (Monteiro et al., 1996 [PMID:8799719]).

HPLC has also been used to simultaneously determine 11 UV-absorbing chemicals, which included bisoctrizole, in sunscreen cosmetics. The limits of quantification and detection were 1700 and 500 ng/mL, respectively, for bisoctrizole (Liu and Wu, 2011 [PMID:21401649]).

Additionally, GC–MS/MS can be used to determine benzotriazoles in various media. For example, headspace solid-phase microextraction followed by GC–MS/MS was used to analyze benzotriazole UV stabilizers in water samples; limits of quantification were below 2 ng/L for drometrizole, allyl-BZT, bumetrizole, ditBu-ClBZT, and ditPe-BZT (Carpinteiro et al., 2010a [PMID:20229350]). In indoor dust, pressurized liquid extraction followed by GC–MS/MS was used; limits of quantification ranged from 4-10 ng/g (Carpinteiro et al, 2010b [PMID:20435314]). In sediments, matrix solid-phase dispersion was used with GC-MS/MS (Carpinteiro et al., 2011 [PMID:21910012]).

Ultrasonic extraction coupled with ultra performance liquid chromatography-photodiode array detector was used for the determination of UV absorbents in plastic food package. Drometrizole, bumetrizole, ditBu-ClBZT, and diMeEtPh-BZT were detected; the limits of detection and quantification ranged from 0.02-0.10 and 0.07-0.35 µg/mL, respectively (Lin et al., 2011).

2.2 Physical-Chemical Properties

The physical-chemical properties for the phenolic benzotriazoles are listed in **Table 2**. When experimental values were not available, predicted values were reported.

Table 2. Physical-Chemical Properties

Chemical	Boiling Point (°C)	Melting Point (°C)	Flash Point* (°C)	Vapor Pressure* (Torr) @ 25 °C	Density (g/cm^3) @ 20 °C and 760 Torr*†	Log P* @ 25 °C	Bioconcentration Factor*∞
P-BZT	407.4±47.0 @ 760 Torr*	127-130 (EtOH) 129-130	200.2±29.3	3.20×10^{-7}	1.33±0.1	3.784±0.737	2.66-312.22
Drometrizole	225	124-133	210.1±31.5	8.79×10^{-8}	1.30±0.1	4.310±1.017	9.39-776.60
tBu-BZT	438.1±55.0 @ 760 Torr*	92.4-93.6 (MeOH) 95-97 (EtOH) 96.5-98.0	218.8±31.5	2.75×10^{-8}	1.18±0.1	5.640±1.022	81.06-7966.11
tBu-ClBZT	465.6±55.0 @ 760 Torr*	120.6-121.8 (MeOH) 121-122.5 (IsoPrOH)	235.4±31.5	2.71×10^{-9}	1.28±0.1	6.331±1.028	188.97-37226.75
Octrizole	471.8±55.0 @ 760 Torr*	104.0-105.2 (MeOH)	239.2±31.5	1.58×10^{-9}	1.10±0.1	7.424±1.027	1862.92-181191.25
EtOH-BZT	501.0±60.0 @ 760 Torr*	n.p.	256.8±32.9	4.71×10^{-11}	1.36±0.1	2.981±0.601	1.45-75.54
Ethanone-BZT	513.2±60.0 @ 760 Torr*	147 (MeOH)	264.2±32.9	3.75×10^{-11}	1.35±0.1	3.783±0.974	1.0-365.80
MaOE-BZT	537.6±60.0 @ 760 Torr*	n.p.	278.9±32.9	3.58×10^{-12}	1.26±0.1	4.622±1.041	8.31-1458.08
Allyl-BZT	450.6±55.0 @ 760 Torr*	100	226.3±31.5	9.75×10^{-9}	1.20±0.1	5.219±1.240	86.74-3882.29
DoM-BZT	545.1±60.0 @ 760 Torr*	n.p.	283.4±32.9	1.71×10^{-12}	1.07±0.1	10.345±1.236	614480.94 (pH10)- 1000000.0 (pH1-9)
sButBu-BZT	458.0±55.0 @ 760 Torr*	81-83 (EtOH)	230.8±31.5	5.22×10^{-9}	1.12±0.1	7.399±0.605	5131.33-158132.05
Bumetrizole	460.4±55.0 @ 760 Torr*	136.2-137.6 (MeOH) 137-141	232.3±31.5	4.24×10^{-9}	1.26±0.1	6.812±1.245	9119.79-86192.72
ditBu-BZT	444.0±55.0 @ 760 Torr*	n.p.	222.3±31.5	1.70×10^{-8}	1.10±0.1	6.853±1.254	11937.77-65864.25
ditBu-ClBZT	469.2±55.0 @ 760 Torr*	147.6-148.8 (MeOH) 154-155.5 154-156 (EtOH)	237.6±31.5	2.00×10^{-9}	1.18±0.1	7.544±1.258	27665.52-310493.53
ditPe-BZT	469.1±55.0 @ 760 Torr	77-79 86.5-88.0 (EtOH)	237.5±31.5	2.01×10^{-9}	1.08±0.1	7.872±1.254	21801.23-395936.69
ditOc-BZT	525.4±60.0 @ 760 Torr*	n.p.	271.5±32.9	1.18×10^{-11}	1.01±0.1	10.736±0.613	1000000.0 (all)
MeEtPhMeBu-BZT	555.5±60.0 @ 760 Torr*	n.p.	289.8±32.9	6.00×10^{-13}	1.07±0.1	9.974±0.611	262354.81 (pH 10)- 1000000.0 (pH 1-9)
MeEtMeBu-CF_3BZT	564.2±60.0 @ 760 Torr*	n.p.	295.0±32.9	2.46×10^{-13}	1.15±0.1	10.025±1.278	121822.15 (pH 10)- 1000000.0 (pH 1-9)
diMeEtPh-BZT	589.3±60.0 @ 760 Torr*	n.p.	310.2±2.9	1.75×10^{-14}	1.12±0.1	9.212±0.610	43581.80-1000000.0
tBuPrAcid-BZT	537.5±60.0 @ 760 Torr*	n.p.	278.9±32.9	2.20×10^{-12}	1.26±0.1	5.149±0.606	1.0-3325.34
tBuPrMeEst-BZT	500.2±60.0 @ 760 Torr*	n.p.	256.3±32.9	1.25×10^{-10}	1.20±0.1	5.569±0.608	1244.59-6925.69
tBuPrHexEst-BZT	864.0±75.0 @ 760 Torr*	n.p.	476.3±37.1	2.18×10^{-31}	1.23±0.1	12.507±0.709	1000000.0 (all)
tBuPrOcEst-BZT	575.1±60.0 @ 760 Torr*	n.p.	301.6±32.9	7.92×10^{-14}	1.11±0.1	9.384±1.246	702286.38 (pH10)- 1000000.0 (pH 1-9)
tBuPrOcEst-ClBZT	596.3±60.0 @ 760 Torr*	n.p.	314.4±32.9	8.14×10^{-15}	1.17±0.1	10.075±1.251	1000000.0 (all)
Bisoctrizole	771.6±70.0 @ 760 Torr*	200	420.5±35.7	1.13×10^{-24}	1.16±0.1	14.347±0.708	1000000.0 (all)

Chemical	Boiling Point (°C)	Melting Point (°C)	Flash Point* (°C)	Vapor Pressure* (Torr) @ 25 °C	Density (g/cm^3) @ 20 °C and 760 Torr*†	Log P* @ 25 °C	Bioconcentration Factor*∞
Oc-NTZ	548.7±60.0 @ 760 Torr*	n.p.	285.7±32.9	1.19×10^{-12}	1.13±0.1	8.608±1.028	15284.07-1000000.0
OcOx-BZT	512.4±60.0 @ 760 Torr*	78-79 (EtOH)	263.7±32.9	4.04×10^{-11}	1.16±0.1	7.744±0.747	1115.42-215606.12

Source: Registry (2010, 2011)
Abbreviations: EtOH = ethanol; IsoPrOH = isopropanol; MeOH = methanol
*calculated properties using Advanced Chemistry Development (ACD/Labs) Software V11.02 (©1994-2010 ACD/Labs)
†when calculated, @ 20 °C and 760 Torr
∞given as values ranging from at pH 10 (low values) to pH 1 (high values) and at 25 °C

Note: The Registry records for tBu(C_{7-9})Est-BZT [127519-17-9], mPEG [104810-48-2], and dPEG [104810-47-1] contained no information on experimental or predicted properties.

2.3 Commercial Availability

Several of the phenolic benzotriazoles are produced primarily by companies in China. Suppliers include those not only in China but also Belgium, Germany, and the United States. The table below lists companies found in BuyersGuideChem, a leading directory of chemical suppliers available online. When the specific product was not found in the directory, additional sources (i.e., in the following order: ChemExper, Chemical Book, and ChemBuyersGuide.com) were then searched for information. No producers or suppliers were located for P-BZT.

Table 3. Producers and Suppliers of Phenolic Benzotriazoles

Chemical	Producers	Suppliers	Source
Drometrizole	*China*: Changzhou Sunlight Pharmaceutical Co., Ltd. Haihang Industry Co., Ltd. Hangzhou Dayangchem Co., Ltd. Hisunny Chemical Co., Ltd. Jinan Great Chemical Co., Ltd. NSTU Chemicals Hangzhou Co. Simagchem Corporation Sinogreat Enterprise Ltd. Tianjin Zhongxin Chemtech Co., Ltd. Xiangyang King Success Fine Chemical Co., Ltd. Yongyi Chemicals Group Co., Ltd. *Germany*: Karl H. Boddin Chemiehandel GmbH [noted as a supplier too] *United States*: Santa Cruz Biotechnology, Inc.	*Belgium*: INNOCHEM *China*: Jinan Haohua Industry Co., Ltd. Kinbester Co., Ltd. Lonwin Industry Group Limited Shanghai Chuangxin Chemicals Co., Ltd. Suzhou Rovathin Pharmatech Co., Ltd. *Germany*: Chemo GmbH Karl H. Boddin Chemiehandel GmbH *United States*: AK Scientific, Inc. BASF Corporation[a] Chemtura Corporation[b] Ciba Specialty Chemicals Corporation[b] Everlight USA, Inc.[a] Kowa American Corporation	BuyersGuideChem (2011a); U.S. EPA (2010a)
tBu-BZT		Germany: Chemos GmbH	BuyersGuideChem (2011b)
tBu-ClBZT		*China*: Apichem Chemical Technology Co., Ltd. Jinan Haohua Industry Co., Ltd. Nanjing Chemlin Chemical Industry Co., Ltd. Simagchem Corporation *United Kingdom*: Leancare Ltd. *United States*: Kingston Chemistry	ChemBuyersGuide.com (undated-a)
Octrizole	*China*: Afine Chemicals Co., Ltd. Changzhou Sunlight Pharmaceutical Co., Ltd. Haihang Industry Co., Ltd. Hangzhou Dayangchem Co., Ltd. Hisunny Chemical Co., Ltd. Jinan Great Chemical Co., Ltd. NSTU Chemicals Hangzhou Co. Shanghai Hanhong Chemical Co., Ltd. Simagchem Corporation Sinogreat Enterprise Ltd. Tianjin Zhongxin Chemtech Co., Ltd. Yongyi Chemicals Group Co., Ltd.	*Belgium*: INNOCHEM *China*: Jinan Haohua Industry Co., Ltd. Kinbester Co., Ltd. Shanghai Trinity Import & Export Co., Ltd. Suzhou Rovathin Pharmatech Co., Ltd. *Germany*: Chemos GmbH *United States*: AK Scientific, Inc. Chemtura Corporation[b] Ciba Specialty Chemicals Corporation[b] Cytec Industries Inc.[b] Mitsubishi Engineered Plastics America[a] Eastar Chemical Corporation	BuyersGuideChem (2011c); U.S. EPA (2010b)

Chemical	Producers	Suppliers	Source
EtOH-BZT		*China*: Apichem Chemical Technology Co., Ltd. Hangzhou Sage Chemical Co., Ltd. HM-Chemo Co., Ltd. *Germany*: Chemical Point *Ukraine*: Enamine Ltd. Ukrorgsynthesis Ltd. *United States*: Kingston Chemistry	ChemBuyersGuide.com (undated-b); ChemExper (2011a)
Ethanone-BZT		*China*: Apichem Chemical Technology Co., Ltd.	ChemBuyersGuide.com (undated-c)
MaOE-BZT	*China*: Jinan Great Chemical Co., Ltd. Shanghai ChemVia Co., Ltd. Yongyi Chemicals Group Co., Ltd.		BuyersGuideChem (2011d)
Allyl-BZT		*China*: Jinan Haohua Industry Co., Ltd.	BuyersGuideChem (2011e)
DoM-BZT	*China*: Jinan Great Chemical Co., Ltd.		BuyersGuideChem (2011f)
sButBu-BZT	*China*: Hangzhou Dayangchem Co., Ltd. Simagchem Corporation Yongyi Chemicals Group Co., Ltd.	*China*: Jinan Haohua Industry Co., Ltd. Suzhou Rovathin Pharmatech Co., Ltd. *Germany*: Beckmann-Kenko GmbH Chemos GmbH	BuyersGuideChem (2011g)
Bumetrizole	*China*: Changzhou Sunlight Pharmaceutical Co., Ltd. Haihang Industry Co., Ltd. Hangzhou Dayangchem Co., Ltd. Hisunny Chemical Co., Ltd. Simagchem Corporation Sinogreat Enterprise Ltd.	*Belgium*: INNOCHEM *China*: Jinan Haohua Industry Co., Ltd. Kinbester Co., Ltd. Lonwin Industry Group Limited Shanghai Chuangxin Chemicals Co., Ltd. Shanghai Trinity Import & Export Co., Ltd. Suzhou Rovathin Pharmatech Co., Ltd. *Germany*: Chemos GmbH *United States*: AK Scientific, Inc. Chemtura Corporation[b] Ciba Specialty Chemicals Corporation[b] Eastar Chemical Corporation Everlight USA, Inc.[a] LG Chem America, Inc.[a] M.Dohmen USA, Inc.[a] NICCA USA, Inc.[a]	BuyersGuideChem (2011h); U.S. EPA (2010c)
ditBu-BZT	*China*: Haihang Industry Co., Ltd. Hangzhou Dayangchem Co., Ltd. Hisunny Chemical Co., Ltd. Jinan Great Chemical Co., Ltd. Shanghai Hanhong Chemical Co., Ltd. Simagchem Corporation Tianjin Zhongxin Chemtech Co., Ltd. *United States*: Santa Cruz Biotechnology, Inc.	*China*: Jinan Haohua Industry Co., Ltd. Kinbester Co., Ltd. Leap Labchem Co., Ltd. Suzhou Rovathin Pharmatech Co., Ltd. *Germany*: Chemos GmbH *United States*: AK Scientific, Inc. Eastar Chemical Corporation	BuyersGuideChem (2011i)

Chemical	Producers	Suppliers	Source
ditBu-ClBZT	*China*: Afine Chemicals Co., Ltd. Changzhou Sunlight Pharmaceutical Co., Ltd. Haihang Industry Co., Ltd. Hangzhou Dayangchem Co., Ltd. Hisunny Chemical Co., Ltd. Jinan Great Chemical Co., Ltd. Shanghai Hanhong Chemical Co., Ltd. Simagchem Corporation Sinogreat Enterprise Ltd. Tianjin Zhongxin Chemtech Co., Ltd. Yongyi Chemicals Group Co., Ltd.	*Belgium*: INNOCHEM *China*: Jinan Haohua Industry Co., Ltd. Kinbester Co., Ltd. Leap Labchem Co., Ltd. Lonwin Industry Group Limited Shanghai Chuangxin Chemicals Co., Ltd. Suzhou Rovathin Pharmatech Co., Ltd. *Germany*: Chemos GmbH *United States*: AK Scientific, Inc. Chemtura Corporation[b] Ciba Specialty Chemicals Corporation[b] Eastar Chemical Corporation LG Chem American, Inc.[a]	BuyersGuideChem (2011j); U.S. EPA (2010d)
ditPe-BZT	*China*: Changzhou Sunlight Pharmaceutical Co., Ltd. Haihang Industry Co., Ltd. Hisunny Chemical Co., Ltd. Jinan Great Chemical Co., Ltd. Shanghai ChemVia Co., Ltd. Shanghai Hanhong Chemical Co., Ltd. Simagchem Corporation Sinogreat Enterprise Ltd.	*Belgium*: INNOCHEM *China*: Jinan Haohua Industry Co., Ltd. Kinbester Co., Ltd. Lonwin Industry Group Limited Shanghai Chuangxin Chemicals Co., Ltd. Suzhou Rovathin Pharmatech Co., Ltd. *Germany*: Connect Chemicals GmbH Klaus F. Meyer GmbH *United States*: 3V Inc.[b] AK Scientific, Inc. BASF Corporation[a] Chemtura Corporation[b] Ciba Specialty Chemicals Corporation[b] Cytec Industries Inc.[b] Eastar Chemical Corporation Everlight USA, Inc.[a]	BuyersGuideChem (2011k); U.S. EPA (2010e)
ditOc-BZT		*China*: Jinan Haohua Industry Co., Ltd. Nanjing Chemlin Chemical Industry Co., Ltd. *United States*: Kingston Chemistry	ChemBuyersGuide.com (undated-d)
MeEtPhMeBu-BZT	*China*: Sinogreat Enterprise Ltd.	*China*: Jinan Haohua Industry Co., Ltd. *Germany*: Chemos GmbH *United States*: Ciba Specialty Chemicals Corporation[b]	BuyersGuideChem (2011l); U.S. EPA (2010f)
MeEtMeBu-CF_3BZT		*China*: Nanjing Chemlin Chemical Industry Co., Ltd. *United Kingdom*: Leancare Ltd. *United States*: Kingston Chemistry	ChemBuyersGuide.com (undated-e)
diMeEtPh-BZT	*China*: Haihang Industry Co., Ltd. Hangzhou Dayangchem Co., Ltd. Hisunny Chemical Co., Ltd. Jinan Great Chemical Co., Ltd. MedicalChem (Yancheng) Manufacturing Co., Ltd. Shanghai Hanhong Chemical Co., Ltd. Simagchem Corporation Sinogreat Enterprise Ltd. Tianjin Zhongxin Chemtech Co., Ltd. *United States*: Santa Cruz Biotechnology, Inc.	*China*: Jinan Haohua Industry Co., Ltd. Kinbester Co., Ltd. Suzhou Rovathin Pharmatech Co., Ltd. *Germany*: Chemos GmbH *United States*: AK Scientific, Inc. Ciba Specialty Chemicals Corporation[b] Eastar Chemical Corporation Everlight USA, Inc.[a]	BuyersGuideChem (2011m); U.S. EPA (2010g)

Chemical	Producers	Suppliers	Source
tBuPrAcid-BZT		*China*: Unispec Chemicals Co.	BuyersGuideChem (2011n)
tBuPrMeEst-BZT		*China*: Hangzhou Sage Chemical Co., Ltd. Nanjing Chemlin Chemical Industry Co., Ltd. *Germany*: ABI Chem *United States*: Ciba Specialty Chemicals Corporation[b] Kingston Chemistry	ChemBuyersGuide.com (undated-f); ChemExper (2011b); U.S. EPA (2010h)
tBuPrHexEst-BZT		*China*: Apichem Chemical Technology Co., Ltd. Hangzhou Sage Chemical Co., Ltd. Nanjing Chemlin Chemical Industry Co., Ltd. *United States*: Kingston Chemistry	ChemBuyersGuide.com (undated-g)
tBuPrOcEst-BZT		*China*: Jinan Haohua Industry Co., Ltd. Nanjing Chemlin Chemical Industry Co., Ltd. Simagchem Corporation *United States*: Kingston Chemistry	ChemBuyersGuide.com (undated-h)
tBuPrOcEst-ClBZT		*Germany*: Chemos GmbH scienTEST	BuyersGuideChem (2011o)
tBu($C_{7\text{-}9}$)Est-BZT	*China*: Haihang Industry Co., Ltd. Hangzhou Dayangchem Co., Ltd. Hisunny Chemical Co., Ltd. Jinan Great Chemical Co., Ltd.	*China*: Jinan Haohua Industry Co., Ltd. Kingreat Chemistry Co., Ltd. *United States*: BASF Corporation[a] Ciba Specialty Chemicals Corporation[b]	BuyersGuideChem (2011p); U.S. EPA (2010i)
Bisoctrizole	*China*: Afine Chemicals Co., Ltd. Haihang Industry Co., Ltd. Hangzhou Dayangchem Co., Ltd. Hisunny Chemical Co., Ltd. Jinan Great Chemical Co., Ltd. Sinogreat Enterprise Ltd. *United States*: Amfine Chemical Corporation [IUR]	*China*: Jinan Haohua Industry Co., Ltd. Kinbester Co., Ltd. Suzhou Rovathin Pharmatech Co., Ltd. *Germany*: Chemos GmbH *United States*: AK Scientific, Inc. Bayer MaterialScience[a] Eastar Chemical Corporation	BuyersGuideChem (2011q); U.S. EPA (2010j)
Oc-NTZ		*China*: Apichem Chemical Technology Co., Ltd. Jinan Haohua Industry Co., Ltd. Nanjing Chemlin Chemical Industry Co., Ltd. Simagchem Corporation *Germany*: Molekula Deutschland Ltd. *Italy*: Allorachem *United Kingdom*: Leancare let. Molekula Ltd. *United States*: Kingston Chemistry	ChemBuyersGuide.com (undated-i); ChemExper (2011c)
OcOx-BZT		*China*: Hangzhou Sage Chemical Co., Ltd. Jinan Haohua Industry Co., Ltd. Nanjing Chemlin Chemical Industry Co., Ltd. Simagchem Corporation *United States*: Kingston Chemistry	ChemBuyersGuide.com (undated-j); ChemExper (2011d); Chemical Book (2008d)

Chemical	Producers	Suppliers	Source
mPEG	*China*: Hangzhou Dayangchem Co., Ltd. Jinan Great Chemical Co., Ltd. Shanghai ChemVia Co., Ltd. Simagchem Corporation Suchem Pharma Co., Ltd.	*China*: Kingreat Chemistry Co., Ltd. Shanghai Sunwise Chemical Co., Ltd.	BuyersGuideChem (2011r)
dPEG	*China*: Changzhou Sunlight Pharmaceutical Co., Ltd. Haihang Industry Co., Ltd. Jinan Great Chemical Co., Ltd. Suchem Pharma Co., Ltd. Yongyi Chemicals Group Co., Ltd.	*China*: Changzhou Sunchem Parmaceutical Chemical Material Co., Ltd. Jinan Haohua Industry Co., Ltd. Kinbester Co., Ltd. Kingreat Chemistry Co., Ltd. Shanghai Chuangxin Chemicals Co., Ltd. Shanghai Sunwise Chemical Co., Ltd. *United States*: AK Scientific, Inc.	BuyersGuideChem (2011s)

[a]2006 Inventory Update Reporting (IUR) Records: importer
[b]2006 IUR Records: not specified as a manufacturer or importer

3.0 Production Processes

Several methods of preparing 2-phenylbenzotriazoles are described by Fukoka et al. (1993 pat.). Overall, previously described methods involve chemical or electrolytic reduction of *o*-nitroazobenzenes. In the present patent, 2-phenylbenzotriazoles (including octrizole) can be prepared by the reduction of an *o*-nitroazobenzene derivative with hydrogen, a hydrogenation catalyst, and a basic substance in an aqueous solvent containing at least one organic solvent (e.g., alcohol, cyclic ether, or aromatic hydrocarbon) (Fukuoka et al., 1993 pat.).

4.0 Production and Import Volumes

The following table provides aggregate U.S. production volumes (in pounds) for several of the benzotriazoles from the IUR database. No data were located for P-BZT, tBu-BZT, tBu-ClBZT, Ethanone-BZT, allyl-BZT, DoM-BZT, MeEtMeBu-CF_3BZT, tBuPrAcid-BZT, tBuPrOcEst-BZT, tBuPrOcEst-ClBZT, Oc-NTZ, and OcOx-BZT. Import volumes were not located.

Chemical	1986	1990	1994	1998	2002	2006
Drometrizole	>1M-10M	>1M-10M	>1M-10M	>1M-10M	>500K-1M	500K-<1M
Octrizole	>500K-1M	>1M-10M	10K-500K	>1M-10M	>1M-10M	1M-<10M
EtOH-BZT	No reports	No reports	<10K	No reports	No reports	No reports
MaOE-BZT	No reports	No reports	<10K	No reports	No reports	No reports
sButBu-BZT	No reports	10K-500K	10K-500K	10K-500K	10K-500K	No reports
Bumetrizole	10K-500K	10K-500K	>500K-1M	>500K-1M	>500K-1M	500K-<1M
ditBu-BZT	No reports	10K-500K	10K-500K	10K-500K	10K-500K	No reports
ditBu-ClBZT	10K-500K	10K-500K	10K-500K	10K-500K	10K-500K	<500K
ditPe-BZT	>1M-10M	>1M-10M	>1M-10M	>1M-10M	>1M-10M	1-<10M
ditOc-BZT	No reports	No reports	10K-500K	No reports	No reports	No reports
MeEtPhMeBu-BZT	No reports	No reports	No reports	No reports	10K-500K	500K-<1M
diMeEtPh-BZT	>1M-10M	>1M-10M	>1M-10M	>1M-10M	>1M-10M	1M-<10M
tBuPrMeEst-BZT	No reports	No reports	10K-500K	>1M-10M	>1M-10M	1M-<10M
tBuPrHexEst-BZT	No reports	10K-500K	No reports	No reports	No reports	No reports
tBu(C_{7-9})Est-BZT	No reports	No reports	>500K-1M	10K-500K	>500K-1M	1M-<10M
Bisoctrizole	No reports	No reports	No reports	No reports	No reports	<500K
mPEG	No reports	10K-500K	No reports	>1M-10M	No reports	No reports

Chemical	1986	1990	1994	1998	2002	2006
dPEG	No reports	10K-500K	No reports	No reports	No reports	No reports

Sources: U.S. EPA (2010a-j, 2011)

5.0 Uses

Phenolic benzotriazoles have been described as "potent UV-light absorbers and constitute an important class of industrial additives for polymers and light-stabilized coatings. They are used in a variety of polymers including polycarbonates, unsaturated polyesters, polystyrenes, acrylics, polyvinyl chloride, thermoplastic polyesters, and polyacetals" (PBA, 2001). Specific examples are briefly provided below.

Octrizole is used as a UV absorber for polymers (ChemicalLand21.com, undated). At a concentration of 1.0 wt.%, it decreased the undesired degradation of bisphenol A polycarbonate by reducing the yellowing index (~2.7 versus 6) and oxidation rate (~0.65 versus 1.0 infrared absorbance at 1713 cm^{-1}) after 870 hours of irradiation (Diepens and Gijsman, 2010). [Note: Data were extracted from figures.]

Drometrizole, ditBu-ClBZT, bumetrizole, and diMeEtPh-BZT are used as UV absorbers in food packaging (Lin et al., 2011). A recent patent application proposes these same chemicals as UV absorbers in personal care products that may be used to treat and/or protect the skin (from burns, cancers, erythema, lentigo, keratotic lesions wrinkles, and cellular changes) and hair (from color changes, embrittlement, tangles, split ends, unmanageability, lack of luster). The product may contain ~0.01-100% of the UV absorber composition and be found in various forms, such as a film or aerosol (Musa and Shih, 2010 pat. appl.). Another patent application proposes use of compositions for controlling, preventing, or treating plant fungi and bacteria with a UV filter that includes benzotriazoles such as drometrizole, ditBu-ClBZT, bumetrizole, ditPe-BZT, diMeEtPh-BZT, OcOx-BZT, and mPEG (Riggs et al., 2010 pat. appl.).

Phenolic benzotriazole are used in a variety of consumer products for various purposes. Octrizole and drometrizole are used as a UV absorber for cosmetic and consumer household products (MakingCosmetics.com Inc., 2009). Octrizole has been identified as a component of Air Wick candles (e.g., AIR WICK® Candles – Magnolia & Cherry Blossom, AIR WICK® Candles Frosted – Vanilla & Soft Cashmere, and AIR WICK® Candles Ribbons – White Berries & Cool Silk) (Reckitt Benckiser, 2010a,b,c). Several issued U.S. patents and patent applications have included the use of octrizole as a sunscreen, UV additive, or UV light stabilizer/absorber. For example, it may be included as an ingredient in top coat nail polish and in an oil-in-water emulsion for use on skin or hair (Holder, 1989 pat.; Hyldgaard et al., 2003 pat.). Octrizole, drometrizole, bumetrizole ditPe-BZT, and tBu(C_{7-9})Est-BZT are also a fragrance ingredient used by International Fragrance Association-affiliated members in consumer goods (IFRA, 2010). According to the Skin Deep Cosmetics Database, some products contain bumetrizole and bisoctrizole. Bumetrizole was identified as an ingredient in a variety of lip products such as lip gloss and lip shine, while bisoctrizole was identified as an ingredient of products containing sunscreen such as moisturizer and day cream (EWG, 2011a,b).

Octrizole is present in Mearlite® Ultra Bright SD, an industrial pigment which may be used to create a simulated pearl finish on alkyd, acrylic, and nitrocellulose. It is present at 5.0-10.0 wt.%

(BASF, 2007, 2010). ditPe-BZT is identified as a component of Olympic Interior/Exterior Varnish (Clear Gloss and Clear Satin) (U.S. DHHS, 2010).

Benzotriazoles are used in dental materials. For example, drometrizole is used in tooth restorative materials while MaOE-BZT can be found in dental pastes (Durner et al., 2010 [PMID:19781758]; Wu et al., 2003 pat. appl.). Additionally, application of MaOE-BZT as a UV absorbent compound occurs in contact lenses (Powell et al., 2006 pat. appl.). Other substituted 2-(2-hydroxyphenyl)benzotriazoles such as Allyl-BZT, 2-(3'-methallyl-2'-hydroxy-5'-methyl phenyl)benzotriazole [also called *ortho*-methallyl Tinuvin P] have also been proposed to be used in ophthalmic lenses or devices (e.g., Jinkerson, 1997 pat.; Your, 2008 pat. appl.).

6.0 Environmental Occurrence and Persistence

6.1 Measurements in Environmental Matrices

Details of environmental occurrence data are provided in Appendix D. Available data were limited. For a better understanding of which chemicals have been found most frequently, this summary is presented on a compound-by-compound basis. It is noted that most of the occurrence data summarized below are not from the United States. [Note: The article by Nakata et al. (2009 [PMID:19806721]) also reports concentrations in marine organisms, such as a lugworm (tidal flat organism), a hammerhead shark (shallow water organism), and coastal birds. Since some of these are species that humans could consume, details regarding these data are located in Section 7.0.]

<u>Drometrizole</u>

Drometrizole concentrations in Spanish raw sewage, Japanese sewage treatment plant effluents (not detected [ND] in the sediments), and Japanese rivers and sediments (whether background or moderately or heavily polluted) were ND to the mid-ppt level (Carpinteiro et al., 2010a [PMID:20229350]; Kameda et al., 2011 [PMID:21429641]). It was found near an outfall of process water discharge from a Japanese paper recycling plant in the water at 13 ppb and at 1.1 ppm in the sediments (Teresaki et al., 2007 [PMID:17941731]). Drometrizole was also detected in leachate from landfills where polyvinyl chloride sheets were used for seepage controls (Fukui et al., 1994). [Note: It was not determined whether drometrizole or other organic substances were solely from the sheets.]

Concentrations of ND to ppb levels were reported in Spanish river and marine sediments and indoor dust from private houses, car cabins, and a public building and in the muscle of many Manila Bay fish species (lipid-weight basis) (Carpinteiro et al., 2010b [PMID:20435314], 2011 [PMID:21910012]; Kim et al., 2011 [PMID:21531423], 2011 in press [PMID:21741069]). Its presence in indoor dust in a German museum storage area was stated to be an artifact (Musshoff et al., 2010 [PMID:20972535]).

In the United States, depending on the core depth and whether the drometrizole was extractable by organic solvents or bound to the sediments, its concentrations in sediments of the Pawtuxet River (1989) and Narragansett Bay (1997) ranged from ND to values in ppb to tenths of a percent (Reddy et al., 2000). Wastewater from a small U.S. specialty chemicals plant contained 0.5-7 ppm drometrizole, while receiving river water contained 0.006-0.10 ppm and its sediments contained 2-670 ppm (Hites et al., 1979; Jungclaus et al., 1978).

Drometrizole was also identified in emissions during heating of nitrogen-containing plastics (e.g., polyurethane and acrylonitrile-butadiene-styrene) at various temperatures; concentrations were 0.015 µg/g on plastic at 100 °C, 1.0 µg/g at 150 °C, 110 µg/g at 200 °C, and 290 µg/g at 300 °C. It was also one of only two nitrogen-containing compounds identified in emissions from polystyrene and polyolefins. Results from the study implied that drometrizole was thermally evaporated from the plastics and released to the working environment and ambient air (Watanabe et al., 2007 [PMID:17383710]).

<u>tBu-BZT</u>

River sediments collected downstream of major cities in the United States and China, and in the vicinity of a specialty chemical plant exhibited levels of the compound that ranged from ND to 60 ppm (Hites et al., 1979; Jungclaus et al., 1978; Zhang et al., 2011 [PMID:21480589]). tBu-BZT levels in water samples also taken in the vicinity of the same specialty chemical plant mentioned above were ND (Hites et al., 1979; Jungclaus et al., 1978). Free and bound Pawtuxent River water sediment levels ranged up to 130 ppm and 260 ppb, respectively (Reddy et al., 2000). Concentration in Chinese sewage sludge collected in 2009 ranged from 0.730 to 1.18 ppb (Zhang et al., 2011 [PMID:21480589]).

<u>tBu-ClBZT</u>

tBu-ClBZT was not found in wastewater discharge or receiving water samples obtained near a small specialty chemical, but the river sediments contained 2-50 ppm (Hites et al., 1979; Jungclaus et al., 1978). In the United States, depending on the core depth and whether tBu-ClBZT was extractable by organic solvents or bound to the sediments, its concentrations in sediments of the Pawtuxet River (1989) ranged from 740 ppb to 71 ppm (Reddy et al., 2000).

<u>Octrizole</u>

Octrizole was sought but ND in the water of Japanese rivers and lakes regardless of pollution level, in Japanese sewage treatment plant (STP) effluents or sediments, or in Australian STP-site groundwater or sewage effluent. It was found in some river and lake sediments in Japan at up to 1.266 ppm, but it was generally in the ND to ppb range. Australian sewage biosolids contained ~123 ppb octrizole (Kameda et al., 2011 [PMID:21429641]; Liu et al., 2011 [PMID:21704319]). Octrizole occurrence in several Manila Bay fish species ranged from ND to the ppb level (Kim et al., 2011 [PMID:21531423], 2011 in press [PMID:21741069]).

<u>Allyl-BZT</u>

Allyl-BZT was sought and ND in raw sewage, indoor dusts, river and marine sediments, and fish muscle (Carpinteiro et al., 2010a [PMID:20229350], 2010b [PMID:20435314], 2011 [PMID:21910012]; Kim et al., 2011 [PMID:21531423]).

<u>Bumetrizole</u>

When found in most media (fish muscle, indoor dust, river and marine sediments, groundwater, sewage influent and effluent, sewage biosolid, sewage sludge), bumetrizole concentrations were generally in the ppb or ppt range (Carpinteiro et al., 2010b [PMID:20435314], 2011 [PMID:21910012]; Kameda et al., 2011 [PMID:21429641]; Kim et al., 2011 [PMID:21531423], 2011 in press [PMID:21741069]; Liu et al., 2011 [PMID:21704319]; Nakata and Shinohara, 2010; Nakata et al., 2009 [PMID:19806721], 2010 [PMID:20959922]; Zhang et al., 2011 [PMID:21480589]). For example, the muscle of multiple Manila Bay fish species (lipid-weight basis) contained bumetrizole in the range ND to 211 ng/g (ppb) lipid weight (Kim et al., 2011 [PMID:21531423], 2011 in press [PMID:21741069]). A single study showed that bumetrizole concentration in the free fraction (defined as removed with organic solvent extraction) from sediment cores from the Pawtuxet River (obtained in 1989) was 260 μg/g (Reddy et al., 2000).

<u>ditBu-BZT</u>

diBu-BZT concentrations in Spanish river and marine sediments; Ariake Sea sediments collected near river mouths, in port, or along the coast of Japan; municipal solid waste refuse-derived fuel (MSW RDF); and the bottom ash and fly ash of an incinerator burning MSW RDF were in the ppb range. Flue gas at the final exit from the incinerator burning MSW RDF was 0.0020 $\mu g/m^3$ (Carpinteiro et al., 2010b [PMID:20435314]; Nakata et al., 2009 [PMID:19806721]; Watanabe and Noma, 2010 [PMID:20227827]). The muscle of multiple Manila Bay fish species (lipid-weight basis) and the blubber of Ariake sea porpoises contained diBu-BZT in the range ND to the ppb level (Kim et al., 2011 [PMID:21531423], 2011 in press [PMID:21741069]; Nakata et al., 2010 [PMID:20959922]). It was not found in a small specialty chemical plant wastewater discharge or receiving water, but the river sediment contained 40 ppm (Hites et al., 1979; Jungclaus et al., 1978).

<u>ditBu-ClBZT</u>

When found in most media (river and marine sediments, sewage influent and effluent, sewage sludge, marine fish muscle lipid, porpoise blubber, MSW RFD, indoor dust, incinerator ashes), ditBu-ClBZT concentrations were ND to the ppb range (Carpinteiro et al., 2010a [PMID:20229350], 2010b [PMID:20435314]; 2011 [PMID:21910012]; Kameda et al., 2011 [PMID:21429641]; Kim et al., 2011 [PMID:21531423], 2011 in press [PMID:21741069]; Nakata et al., 2010 [PMID:20959922]; Watanabe and Noma, 2010 [PMID:20227827]; Zhang et al., 2011 [PMID:21480589]). While not found in a small specialty chemical plant wastewater discharge or receiving water, the river sediments contained 2-300 ppm ditBu-ClBZT (Hites et al., 1979; Jungclaus et al., 1978). It was also found at the ppm level in sediments of Narragansett Bay and the Pawtuxet River, with values ranging up to 0.52% in the latter (Reddy et al., 2000).

<u>ditPe-BZT</u>

When found in most media (fish muscle, indoor dust, river and marine sediments, water, sewage influent and effluent), ditPe-BZT concentrations were generally in the ppb or ppt range (Carpinteiro et al., 2010b [PMID:20435314], 2011 [PMID:21910012]; Kameda et al., 2011 [PMID:21429641]; Kim et al., 2011 [PMID:21531423], 2011 in press [PMID:21741069]; Nakata and Shinohara, 2010; Nakata et al., 2009 [PMID:19806721]; Zhang et al., 2011 [PMID:21480589]). For example, ditPe-BZT concentrations in sediment obtained from the Ariake Sea ranged from 2.8 to 320 ng/g dry wt. (Nakata et al., 2009 [PMID:19806721]). Studies indicated that ditPe-BZT was present in river waters as well as associated river sediments obtained in Japan; sediment concentrations of ditPe-BZT were generally greater in river sediment samples (Kameda et al., 2011 [PMID:21429641]).

diMeEtPh-BZT

The muscle of multiple Manila Bay fish species (lipid-weight basis) contained diMeEtPh-BZT in the range ND to 62.9 ng/g lipid weight (Kim et al., 2011 [PMID:21531423], 2011 in press [PMID:21741069]). Of the tested fish, the compound was detected in 55% of analyzed specimens (Kim et al., 2011 in press [PMID:21741069]). While not detected in surface waters (rivers and streams) or sewage effluents, diMeEtPh-BZT was detected in sediment samples obtained close to the surface water sampling sites. Sediment concentrations ranged from ND to 1266 μg/kg (Kameda et al., 2011 [PMID:21429641]).

sButBu-BZT

In a flow-through 60-day fish bioconcentration assay, conducted according to the Organisation for Economic Co-operationa nd Development Guideline 305, the carp (*Cyprinus carpio*) bioconcentration factors for sButBu-BZT after 60 days were 7,700 at ambient water concentration 1 μg/L and 13,000 (at 0.1 μg/L). During the 32-day depuration period, the compound was rapidly excreted. The half-life was approximately 14 days. Concentrations in integument, head, and viscera at 60 days were 7,490-24,400 ng/g, while concentrations in the remaining parts were 4,610-9.590 ng/g at a water concentration of 1 μg/L. At a lower concentration (0.1 μg/L), the values were 965-3,820 and 665-868 ng/g, respectively (Ciba Specialty Chems, 2001).

Mixture mPEG/dPEG [Tinuvin 1130 Tested]

In an earlier Japanese bioaccumulation test with carp, the commercial mixture was not bioaccumulated at water concentrations of 1.0 and 0.1 ppm (wt/vol). The HPLC limit of determination in the fish was 0.23 ppm (Ciba-Geigy Corporation, 1986a). In a modified Sturm test, Tinuvin 1130 was identified as not being readily biodegradable (Ciba-Geigy Corp., 1987).

6.2 PBT Profiler Data

The PBT Profiler has estimated that most of the phenolic benzotriazoles is expected to be found predominantly in soil and sediment. Predicted half-lives ranged from 0.075 days (air) to 1600 days (sediment), while bioconcentration factors (BCFs) ranged from 3.1 to 10,000 (U.S. EPA, 2010k).

Chemical*	Media Half-Life [days] (Percent in Medium)				BCF	Fish Chronic Toxicity Value (mg/L)
	Water	Soil	Sediment	Air		
P-BZT	15 (19)	30 (81)	140 (0)	0.62 (0)	19	0.006
Drometrizole	38 (10)	75 (84)	340 (5)	0.54 (0)	320	0.007
tBu-BZT	38 (10)	75 (84)	340 (6)	0.54 (0)	350	0.008
tBu-ClBZT	60 (6)	120 (75)	540 (19)	0.54 (0)	930	0.009
Octrizole	60 (2)	120 (47)	540 (51)	0.5 (0)	5800	0.003
EtOH-BZT	15 (23)	30 (77)	140 (0)	0.46 (0)	5.6	0.008
Ethanone-BZT	38 (21)	75 (79)	340 (0)	0.71 (0)	3.1	0.008
MaOE-BZT	38 (11)	75 (87)	340 (2)	0.24 (0)	180	0.009
Allyl-BZT*	38 (10)	75 (84)	340 (6)	0.27 (0)	370	0.008
DoM-BZT	38 (2)	75 (39)	340 (59)	0.5 (0)	370	not estimated
sButBu-BZT	38 (2)	75 (45)	340 (53)	0.92 (0)	6700	0.003
Bumetrizole	60 (4)	120 (60)	540 (36)	1.1 (0)	1300	0.009
ditBu-BZT	60 (2)	120 (47)	540 (51)	1.2 (0)	3800	0.003

Chemical*	Media Half-Life [days] (Percent in Medium)				BCF	Fish Chronic Toxicity Value (mg/L)
	Water	Soil	Sediment	Air		
ditBu-ClBZT	60 (1)	120 (43)	540 (55)	1.2 (0)	10,000	0.0011
ditPe-BZT	60 (1)	120 (43)	540 (56)	1 (0)	6000	0.00064
ditOc-BZT	180 (1)	360 (52)	1600 (48)	0.96 (0)	280	not estimated
MeEtPhMeBu-BZT	180 (1)	360 (52)	1600 (47)	0.83 (0)	1000	not estimated
MeEtMeBu-CF_3BZT	180 (1)	360 (51)	1600 (49)	0.88 (0)	340	not estimated
diMeEtPh-BZT	60 (1)	120 (42)	540 (57)	0.75 (0)	3700	0.00041
tBuPrAcid-BZT	38 (12)	75 (87)	340 (1)	0.96 (0)	3.2	0.099
tBuPrMeEst-BZT	38 (8)	75 (75)	340 (17)	1 (0)	510	0.01
tBuPrHexEst-BZT	38 (2)	75 (41)	340 (58)	0.71 (0)	1300	0.00062
tBuPrOcEst-BZT*	38 (2)	75 (40)	340 (58)	0.62 (0)	430	not estimated
tBuPrOcEst-ClBZT	60 (1)	120 (42)	540 (57)	0.16 (0)	210	not estimated
tBu($C_{7\text{-}9}$)Est-BZT	60 (1)	120 (42)	540 (57)	0.62 (0)	3200	0.00032
Bisoctrizole	180 (1)	360 (52)	1600 (47)	0.5 (0)	28	not estimated
Oc-NTZ	60 (1)	120 (42)	540 (56)	0.5 (0)	8600	0.00055
OcOx-BZT	38 (3)	75 (49)	340 (47)	0.075 (0)	170	0.005

*Data were not available for mPEG or dPEG.

7.0 Human Exposure

Based on their use in a variety of consumer products (e.g., candles and cosmetics), human exposure may occur through oral or dermal exposure and inhalation.

General Population Exposure

Bisoctrizole was determined in 100 sunscreen cosmetics at concentrations ranging from 0.10% to 1.97%; the maximum allowed concentration is 10% (Liu and Wu, 2011 [PMID:21401649]). The Skin Deep Cosmetic Safety Database listed products (e.g., lip gloss, and moisturizer) that contained bumetrizole and bisoctrizole. [See Section 5.0.]

Exposure may occur from the consumption of marine organisms. Bumetrizole, ditBu-BZT, ditBu-ClBZT, and ditPe-BZT were found in a number of tidal flat and shallow water organisms collected from the Ariake Sea in Japan. For example, concentrations (ng/g wet weight) in oysters ranged from 0.36 (ditBu-BZT) to 2.2 (ditPe-BZT), while those in clams were 0.45 (ditBu-BZT) to 1.3 (bumetrizole); both species were tidal flat organisms. Generally, concentrations of UV stabilizers were greater in organisms from tidal flat than in those from shallow water. For instance, the following concentrations (ng/g wet weight) were reported in shrimp: ditBu-BZT, 0.21 (tidal) and <0.05 (shallow water); bumetrizole, <0.01 (tidal) and 0.32 (shallow water); ditBuCl-BZT, 0.87 (tidal) and 0.52 (shallow water); ditPe-BZT, 0.35 (tidal) and 0.20 (shallow water) (Nakata et al., 2009 [PMID: 19806721]).

Human exposure may occur through migration from polycarbonate containers that are intended for use in microwave ovens. Octrizole was present in a methanol extract from a polycarbonate container dissolved in dichloromethane. The calculated potential migration of octrizole was 4.1 µg/g food (Nerin et al., 2003 [PMID:12952414]).

Additionally, exposure is possible from tooth restorative materials. In a study of methanolic eluates from polymerized specimens (mp) and methanolic eluates from unpolymerized specimens (mu), the following amounts of drometrizole (referred to an internal caffeine [CF] standard, where 0.1 mg/mL CF = 100%): 34 and 36%CF in the mp and mu of Tetric® composite, respectively; 15 and 308 %CF in mp and mu of Arabesk® composite, respectively; and 7.7 and 89%CF of mp and mu of Admira® ormoceres, respectively (Durner et al., 2010 [PMID:19781758]).

Occupational Exposure

The National Institute for Occupational Safety and Health (NIOSH) National Occupational Exposure Survey (1981-1983) statistically estimated the number of workers exposed to a few phenolic benzotriazoles. The total number of workers exposed, number of female workers exposed, and the occupation with the greatest number of total exposed workers reported is presented in **Table 4**.

Table 4. NIOSH National Occupational Exposure Survey Data

Chemical	Total Number of Workers	Total Number of Female Workers	Occupation Description with the Greatest Number of Exposed Workers	Reference
Drometrizole	52,370	21,694	Molding and casting machine operators	NIOSH (undated-a)
Octrizole	21,108	9686	Molding and casting maching operators	NIOSH (undated-b)
ditBu-ClBZT	5246	3148	Machine operators, not specified	NIOSH (undated-c)
ditPe-BZT	973	95	Painting and paint spraying machine operators	NIOSH (undated-d)

More recent information regarding worker exposure has been compiled in the 2006 IUR Records. **Table 5** displays the information available for several phenolic benzotriazoles.

Table 5. Manufacturing, Processing, and Use Worker Information

Chemical	Number of Workers	Number of Sites	Reference
Drometrizole	≥1000	100-999	U.S. EPA (2010a)
Octrizole	≥1000	≥1000	U.S. EPA (2010b)
Brumetrizole	100-999	1-99	U.S. EPA (2010c)
ditBu-ClBZT	100-999	1-99	U.S. EPA (2010d)
ditPe-BZT	≥1000	100-999	U.S. EPA (2010e)
MeEtPhMeBu-BZT	100-999	1-99	U.S. EPA (2010f)
diMeEtPh-BZT	≥1000	100-999	U.S. EPA (2010g)
tBuPrMeEst-BZT	100-999	1-99	U.S. EPA (2010h)
tBu(C_{7-9})Est-BZT	≥1000	100-999	U.S. EPA (2010i)
Bisoctrizole	1-99	1-99	U.S. EPA (2010j)

[a]Aggregated Number of Reasonable Likely to be Exposed Industrial Manufacturing, Processing, and Use Workers
[b]Aggregated Number of Manufacturing, Processing, and Use Sites

8.0 Regulatory Status

Drometrizole, tBu-BZT, octrizole, EtOH-BZT, MaOE-BZT, sButBu-BZT, ditBu-BZT, ditPe-BZT, ditOc-BZT, MeEtPhMeBu-BZT, MeEtMeBu-CF_3BZT, diMeEtPh-BZT, tBuPrMeEst-BZT, tBuPrHexEst-BZT, tBuPrOcEst-ClBZT, tBu(C_{7-9})Est-BZT, bisoctrizole, Oc-NZT, mPEG, and dPEG are listed on the U.S. Environmental Protection Agency (EPA) Toxic Substances Control Act Inventory (U.S. EPA, 2010l). Drometrizole, octrizole, DoM-BZT, bumetrizole, ditPe-BZT, tBuPrMeEst-BZT, tBu(C_{7-9})EST-BZT, and mPEG/dPEG are also regulated by the EPA as an inert ingredient that is permitted for use in nonfood use pesticide products (U.S. EPA, 2010m). In effect on August 18, 2010, both DoM-BZT and ditPe-BZT are exempted from the requirement of a tolerance when used as an inert ingredient (i.e., UV stabilizer at a maximum concentration of 0.06%) in insecticide formulations applied before harvest to several plants such as canola, chickpeas, cotton, navy beans, lentils, sunflower (U.S. EPA, 2010n). In 1994, the EPA revoked a Significant New Use Rule (SNUR) for tBu(C_{7-9})Est-BZT that was promulgated in 1993 based on the conclusion that the chemical would not present an unreasonable risk to health (U.S. EPA, 1994). In 1998, an SNUR for MaOE-BZT was modified (U.S. EPA, 1995, 1998).

Under the U.S. Food and Drug Administration, drometrizole, octrizole, bumetrizole, and diMeEthPh-BZT are approved for use as an antioxidant/stabilizer for polymers under specifically noted limitations [21CFR178.2010] (U.S. FDA, 2011a). ditPe-BZT is approved for use as a component of food packaging adhesives [21CFR175.105] (U.S. FDA, 2011b).

As a food contact substance, the Office of Food Additive Safety has established the following dietary concentration and cumulative estimated daily intake levels:

Chemical	Dietary Concentration (ppb)	Cumulative Estimated Daily Intake (mg/kg body weight/day)	Reference
Drometrizole	0.0029	0.15	U.S. FDA (2011c)
Octrizole	0.06	0.000003	U.S. FDA (2011d)
Bumetrizole	5	0.00025	U.S. FDA (2011e)
ditBu-ClBZT	0.4	0.00002	U.S. FDA (2011f)
ditPe-BZT	7	0.00035	U.S. FDA (2011g)
diMeEtPh-BZT	22	0.0011	U.S. FDA (2011h)
Bisoctrizole	4.5	0.000225	U.S. FDA (2011i)

Drometrizole, octrizole, sButBu-BZT, bumetrizole, ditBu-BZT, ditBu-ClBZT, ditPe-BZT, MeEtPhMeBu-BZT, diMeEtPh-BZT, tBu(C_{7-9})Est-BZT, bisoctrizole, mPEG, and dPEG are specified on the Domestic Substances List (published May 4, 1994) (Environment Canada, 2011). Under the Registration, Evaluation, Authorisation and Restriction of Chemicals Regulation, octrizole, sButBu-BZT, ditBu-BZT, ditBu-ClBZT, and ditPe-BZT are each listed as a high-priority substance for further investigation (Environment Agency, 2010).

9.0 Toxicological Data

9.1 General Toxicology

A summary of the available toxicological data for phenolic benzotriazoles is provided in the table below. If the chemical is not listed in the table below, no toxicological data were located. Detailed information and results are provided in the sections following the table.

Chemical	CASRN	Human Data	Chemical Disposition, Metabolism, and Toxicokinetics	Acute Toxicity	Subchronic Toxicity	Chronic Toxicity	Cytotoxicity	Reproductive and Teratological Toxicity	Carcinogenicity	Genotoxicity	Other Data
Drometrizole	2440-22-4	X		X	X	X	X	X	X	X	X
Octrizole	3147-75-9	X		X	X					X	X
Bumetrizole	3896-11-5									X	X
ditBu-BZT	3846-71-7			X	X	X		X		X	
ditBu-ClBZT	3864-99-1				X			X		X	X
ditPe-BZT	25973-55-1			X	X			X		X	X
diMeEtPh-BZT	70321-86-7			X	X			X		X	X
Bisoctrizole	103597-45-1	X		X							X
tBuPrAcid-BZT	84268-36-0		X		X		X				X
tBuPrMeEst-BZT	84268-33-7		X		X						
tBuPrHexEst-BZT	84268-08-6		X		X						
mPEG/dPEG (Tinuvin 1130)*	104810-48-2/ 104810-47-1		X	X	X			X		X	X

*Studies with Tinuvin 1130 were included under this heading since the main components of the mixture were mPEG and dPEG. See footnotes under select tables for further details.

9.1.1 Human Data

A repeat insult patch test on volunteers using octrizole was negative for skin sensitization (Cytec, 1999). Drometrizole was proposed to induce contact allergy in 1 of 33 patients with suspected contact dermatitis (Tomar et al., 2005 [PMID:16471456]).

Tinosorb® M (active ingredient: bisoctrizole), however, has caused allergic contact dermatitis in two individuals. One case involved a 75-year-old nonatopic male with an eczematous eruption 1-2 days after application of sunscreen. The second case involved an 85-year-old female who had eczematous changes mostly on the face, neck, and arms for over 13 years. Both patients had positive reactions to Tinosorb® M in both the irradiated and non-irradiated test series (O'Connell et al., 2011). In two 52-year-old males (one Caucasian, one African American) experiencing atopic dermatitis since childhood and who had developed a persistent pruritic photosensitive eczematous eruption, phototest results were interpreted as chronic actinic dermatitis. Photopatch tests were then performed; positive results suggested both an allergic contact dermatitis and photoallergic contact dermatitis to bisoctrizole. Exposure to the chemical may have occurred from use of one of the many sunscreens (Gonzalez et al., 2011 [PMID:21504696]). Similarly, a previous case report discussed development of allergic contact dermatitis in a 54-year-old woman after using sunscreen containing bisoctrizole (Gonzalez-Perez et al., 2007 [PMID:17244092]). Another earlier case report discussed development of contact allergic reaction in 67-year-old man using the sunscreen product Lait Avene 60 (60B/60A) which contained 6% Tinosorb® M (Andersen and Goossens, 2006).

9.1.2 Chemical Disposition, Metabolism, and Toxicokinetics

In vitro studies with tBuPrMeEst-BZT showed that it was hydrolyzed by rat serum (apparent K_m = 0.13 mM, apparent V_{max} = 1.13 µmol/min × mL) and rat liver homogenates (apparent K_m = 0.15 mM, apparent V_{max} = 0.5 µmol/min × g). Metabolism by rat small intestine homogenates was less efficient than observed using liver homogenates (apparent K_m = 0.49 mM, apparent V_{max} = 0.000215 µmol/min × g). Metabolism of mPEG/dPEG was reduced compared to tBuPrMeEst-BZT using all three biological sources ($V_{0.2mM}$ ranged from below detection limit to 0.000175 µmol/min × g) (Thomas et al., 1995).

Male rats (n=2) were orally dosed with 10 mg/kg tBuPrMeEst-BZT or tBuPrHexEst-BZT. Maximal blood concentration of tBuPrMeEst-BZT (1.675 and 1.866 μg_{pe}/g) was achieved between 1 and 2 hours. The apparent half-life was less than 12 hours and minimal amount remained 48 hours after dosing. tBuPrAcid-BZT appeared to be the major metabolite formed through hydrolysis of the parent compound. Compared to the high absorption of tBuPrMeEst-BZT, tBuPrHexEst-BZT was lower (C_{max} = 0.122 and 0.103 μg_{pe}/g). The apparent half-life was ~12 hours. Hydrolysis of tBuPrHexEst-BZT played a major role in metabolism (Thomas et al., 1995).

9.1.3 Acute Exposure

The oral LD_{50} values for chemicals with available data were ≥1000 mg/kg in mice and rats. Dermal LD_{50} values, obtained from three chemicals, were >2000 mg/kg in rats and >5000 mg/kg in rabbits. Inhalation LC_{50} values in rats were >1420 mg/m^3 and >50 mg/L.

Chemical	CASRN	LD_{50} (oral)*	LD_{50} (dermal)*	LC_{50}*	Reference(s)
Drometrizole	2440-22-4	6500 mg/kg (mouse) >10,000 mg/kg (M& F Tif: RAIf (SPF) rat) >5000 mg/kg (mouse)		>1420 mg/m^3 (M&F rat)	ChemIDplus (undated); U.S. EPA (2010o)
Octrizole	3147-75-9	1000 mg/kg (rat) >10,000 mg/kg (mammalian)	>5000 mg/kg (rabbit)	>50 mg/L (rat)	U.S. EPA (2010p); Cytec (1999); U.S. EPA (2004)
ditBu-BZT	3846-71-7	>2000 mg/kg (M&F CD(SD)IGS rat)			Hirata-Koizumi et al. (2009a [PMID:20021483])
ditPe-BZT	25973-55-1	>2325 mg/kg (M& F Tif: RAIf (SPF) rat)			U.S. EPA (2010q)
diMeEtPh-BZT	70321-86-7	>7750 mg/kg (M& F Tif: RAIf (SPF) rat)	>2000 mg/kg (M&F rat)		U.S. EPA (2010r)
Bisoctrizole	103597-45-1	>2000 mg/kg (rat)	>2000 mg/kg (rat)		RTECS (2006)
Tinuvin 1130†		>5000 mg/kg (M&F Tif:RAIf (SPF) rat)	>2000 mg/kg (M&F Tif:RAIf (SPF) rat)		Ciba-Geigy Corporation (1987, 1992a)

*Unless noted, the strain and/or sex of tested animals was not provided.
†One of the noted references did not provide information on the composition of the test substance (Ciba-Geigy Corporation, 1987). Another stated that the test substance was a reaction mixture (trade names Tinuvin 213 and Tinuvin 1130) containing 50-60% mPEG, 30-35% dPEG, and 12-15% polyethylene glycol (Ciba-Geigy Corporation, 1992a).

Abbreviations: F = female(s); LC_{50} = lethal concentration for 50% of test animals; LD_{50} = lethal dose for 50% of test animals; M = male(s)

9.1.4 Short-Term and Subchronic Exposure

Overall, oral exposure (either through gavage or in feed) of the tested chemicals to rats led to liver effects. Increased absolute and/or relative liver weights were observed in several studies. Body weight and body weight gain changes were observed after administration of several test substances. Histopathological changes (e.g., foci, hypertrophy, and cytoplasmic vacuolization) and altered liver enzyme content and activities were also noted after treatment with different phenolic benzotriazoles. Hematological effects (e.g., altered white and red blood cell counts, altered albumin levels, and packed cell volume) were observed. For those studies that calculated no observed adverse effect levels (NOAELs), the values ranged from <0.5 to ~5685 mg/kg/day.

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
Drometrizole	2440-22-4	Rat, albino RAI, age n.p., 10M/dose	Orally gavaged with 300 mg/kg/day; two groups treated for 14 and 28 days and killed one day after final dose, third group treated 14 days and killed after a 28-day recovery period	Significant increase in relative liver weights was noted in all three groups. No effects on body weight gain were noted. Significant increase in aminopyrine *N*-demethylase activity was observed after 28 day treatment and UDP glucuronosyltransferase activity was increased after 14 and 28 days of treatment. Glucose 6-phosphatase activity was decreased after 14 days of treatment.	CIR Expert Panel (2008 [PMID:18569163]; Schmid et al. (1980 [PMID:7419140])
		Rat, strain, age, number, and sex n.p.	Orally dosed for 90 days	Effects observed included changes in liver weight, changes on white blood cell count, and changes in testicular weight. The TD_{Lo} was 270 mg/kg.	RTECS (2010)
Octrizole	3147-75-9	Rat, Wistar, age n.p., 5M and 5F/dose	Orally dosed 1.25, 2.5, or 5% (1.286, 2.594, and 5.658, respectively) for 30 days	No deaths or abnormal appearance or behaviors were noted during the dosing period. Hydronephrosis was observed in three controls and four animals in the high-dose group. [Note: The sex of the affected animals was not provided. Additionally, it was noted that hydronephrosis was common in these animals.] No lesions associated with dosing were observed. The NOAEL was 5.685 g/kg/day.	U.S. EPA (2010p)

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
ditBu-BZT	3846-71-7	Rat, Crj;CD(SD) IGS; 5 weeks old, 5-10/sex/dose, M&F	Orally gavaged with 0.5, 2.5, 12.5, or 62.5 mg/kg/day for 28 days; 5 rats at highest dose were kept for a 14-day recovery period and then killed	No death or clinical toxicity signs were noted. A significant increase in food consumption on dosing days 14 and 21 in M and 21 and 27 in F was noted at the highest dose. However, no effects on body weight were observed. Significant decreases in red blood cell count, hematocrit, and hemoglobin were observed at doses ≥2.5 mg/kg. Mean corpuscular hemoglobin concentration was decreased at ≥12.5 mg/kg in M. Significant increase in platelet count was noted at the highest dose in M. A significant decrease in fibrinogen occurred at ≥2.5 mg/kg in M and 62.5 mg/kg in F. Blood biochemical effects (e.g., albumin and total cholesterol) were noted at ≥0.5 mg/kg in M and 62.5 mg/kg in F. Absolute liver weight was increased at ≥2.5 mg/kg in M and ≥12.5 mg/kg in F, while relative weight was increased at all doses in M and at ≥12.5 mg/kg in F. Increased absolute and relative M kidney weight and absolute F heart weight were also increased at the highest dose tested. Histopathological evaluations indicated changes in liver, heart, kidneys, thyroids, and spleen; effects typically occurred at lower doses in M. After the recovery period, changes mostly recovered in F. The NOAEL was <0.5 mg/kg/day in M and 2.5 mg/kg/day in F.	Hirata-Koizumi et al. (2007 [PMID:17934922])

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
ditBu-BZT	3846-71-7	Rat, Crl:CD(SD); 4 weeks old (treated at 5 weeks old), 4/sex/dose, M&F	Orally gavaged with 0.5, 2.5, or 12.5 mg/kg/day for 28 days	Increased body weight was observed in M administered 0.5 mg/kg on day 14. No other clinical signs of toxicity were observed. Enlarged liver was noted in all M at doses ≥2.5 mg/kg and in a single M given 0.5 mg/kg. A single F showed liver enlargement at the highest dose tested. Increased absolute and relative liver weights were noted in M at doses ≥2.5 mg/kg and F at 12.5 mg/kg. White foci in the liver were noted in M and F at same doses that produced effects on liver weights. Total cytochrome P450 liver content was increased in M at doses ≥2.5 mg/kg. Select enzyme activities were also altered (e.g., EROC activity decreased in all M dose groups, testosterone 2α- and 16α-hydroxylase activity decreased in M in mid and high dose groups). Compound was rapidly absorbed and eliminated; peak plasma levels occurred <10 hours after dosing. No gender related differences were noted in the plasma profiles of either sex. Metabolites were not detected in blood.	Hirata-Koizumi et al. (2009b [PMID:19538016])
		Rat, Crl:CD(SD), 11 weeks old (M) and 10 weeks old (F) mated Sex of pups determined on postnatal day 4, 10/sex/dose, M&F	Orally gavaged pups with 0.1, 0.5, 2.5, or 12.5 mg/kg/day on postnatal days 4-21	No clinical signs of toxicity or effects on body weight gain. Blood biochemical effects (e.g., albumin and blood urea nitrogen) were noted at the highest dose tested in both sexes. Increased relative liver weights occurred in both sexes at doses ≥2.5 mg/kg. Histopathological changes noted (e.g., hypertrophy, anisokaryosis and/or nucleolar enlargement) occurred in both sexes at doses ≥2.5 mg/kg.	Hirata-Koizumi et al. (2007 abstr.; 2008a [PMID:18330788])
		Rat, castrated Crl:CD(SD), 6 weeks old, 10/sex/dose, M&F	Orally gavaged with 0.5, 2.5, or 12.5, mg/kg/day for 28 days	No death or clinical toxicity signs were noted. No changes in body weight or food consumption. Blood biochemical changes occurred in both sexes starting at 0.5 mg/kg. Absolute and relative liver weights were increased at ≥0.5 mg/kg in M and 12.5 mg/kg in F. Histopathological changes occurred at ≥0.5 and ≥2.5 mg/kg in M and F, respectively.	Hirata-Koizumi et al. (2008b [PMID:18161511])

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
ditBu-BZT	3846-71-7	Rat, Crl:CD(SD) IGS, 5 weeks old (6 weeks old at treatment), 20/sex/dose, M&F	M orally gavaged with 0.1, 0.5, or 2.5 mg/kg and F with 0.5, 2.5, or 12.5 mg/kg for 13 weeks	One M rat given 2.5 mg/kg was found dead on day 54. Increased osmotic pressure and specific gravity were detected in urine of high-dose M. Hematological effects were noted at ≥0.5 and 12.5 mg/kg in M and F, respectively. Enlarged livers were noted at 2.5 and 12.5 mg/kg in M and F, respectively; histopathology showed centrilobular hypertrophy of hepatocytes with eosinophilic granular cytoplasm. Increased absolute and relative liver weights were noted in M and F at ≥0.5 and 12.5 mg/kg, respectively. Increased relative brain, heart, kidneys, and testes weights were noted in high-dose M.	Hirata-Koizumi et al. (2008d [PMID:18161509])
ditBu-ClBZT	3864-99-1	Rat, Crj:CD(SD) IGD; 11 weeks old (M) and 10 weeks old (F), 10 or 15/sex/dose, M&F	Orally gavaged with 2.5, 25, or 250 mg/kg/day starting 28 days prior to mating: M were dosed for 56-57 days and F were dosed 55-69 days (through lactation day 3). M euthanized on day 56-57 and F either euthanized on days 4-6 after parturition or were kept for an additional 14-day recovery period.	No deaths were noted in M or F. No effects on body weight, food consumption, or general condition were observed. Increased albumin, albumin/globulin ratio, and alkaline phosphatase levels were observed in M at ≥25 mg/kg. Increased absolute and relative liver weights in M were also observed at doses ≥25 mg/kg. No changes were reported in F. Histopathological evaluations were negative in both sexes. The results indicated that M rats have >100× higher susceptibility to the substance than F.	Ema et al. (2008 [PMID:18622873])
		Rat, strain, age, number, and sex n.p.	Oral administration for 90 days	Changes noted included altered liver weight, impaired liver function tests, and other liver effects [not described]. The TD_{Lo} was 81 mg/kg.	RTECS (2000)

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
ditBu-ClBZT	3864-99-1	Rat, Crl:CD(SD), 11 weeks old (M) and 10 weeks old (F), 6/sex/group, M&F After 7-day acclimation, F cohabitated with 1 M. 12 pregnant rats were assigned each for the castration and preweaning study. On gestation day 20, pregnant F were separated and allowed to deliver spontaneously. After weaning on postnatal day 21, half of M and F pups in good health were castrated and treated at 6 weeks old.	Orally gavaged with 250 mg/kg/day for 28 days	*Intact Rats* No deaths or clinical signs of toxicity were observed. M body weight gains during the administration period were significantly increased compared to controls. Food consumption was also significantly increased on certain days. F body weight gain was markedly increased on days 0-4, decreased on days 4-7, and increased on days 11-14. No difference in food consumption was noted between treated and control F. M rats had increased relative liver weight that was twice that of controls; in F, the rate of change was <10%. Hypertrophy, decreased glycogen, and eosinophilic granular change were seen in M rat hepatocytes only. *Castrated Rats* No deaths or clinical signs of toxicity were observed. Body weight gain was markedly increased on day 21-25 in M and decreased on days 4-7 in F. No difference in food consumption was noted in either sex. M had a significant increase in absolute and relative liver weight (~40%) compared to controls. Both sexes exhibited no histopathological changes in the liver. *Conclusion* Castration significantly reduced the gender-related difference seen above regarding toxicity (including hepatotoxicity).	Hirata-Koizumi et al. (2008c [PMID:18622872])
		Rats (preweaning), 16/sex/group, M&F	Orally gavaged with 250 or 500 mg/kg/day on postnatal days 4-21	No deaths or clinical signs of toxicity were observed. A significantly decreased body weight gain during the treatment period, biochemical changes (e.g., increase in aspartate aminotransferase levels and decrease in glucose levels), increase in several organ weights (e.g., absolute and relative liver weight and absolute heart weight), and histopathological changes in the liver (e.g., hypertrophy) were observed in both sexes at both doses.	Hirata-Koizumi et al. (2008c [PMID:18622872])

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
ditPe-BZT	25973-55-1	Rat, Wistar, newly weaned, 20/sex/dose, M&F	100, 200, 400, 800, or 1600 ppm in food for 90 days	No deaths were reported. At the high dose, body weight gain and food consumption were decreased. M exhibited a treatment-related decrease of hemoglobin content and packed cell volume in M at ≥200 ppm; this was less evident in F. There was an increase in glucose-6-phosphatase at lower dose groups with a steady-state level at ~200 ppm. Liver, kidney, spleen, and testes weights were increased. At the high dose, increased thyroid weights were also observed. The liver had a greenish-drab discoloration in M and F at higher dose levels. Foci of necrosis, slight proliferation of bile duct epithelia, and enlarged parenchymal cells were observed. M given higher doses had tubular necrosis in the kidneys, while F had treatment-related, yellowish-brown pigmentation in the cytoplasm of the proximal tubular cells. The NOEL was <100 ppm and the NOAEL was 100 ppm (~22 mg/kg body weight/day).	U.S. EPA (2010q)
diMeEtPh-BZT	70321-86-7	Rat, Tif:RAIF (SPF) albino, ~4 weeks old, 40/sex/dose, M&F	50, 300, 2000, or 10,000 ppm in food for 92-94 days	No deaths occurred and no signs of toxicity were observed. Statistically significant increase in mean liver weight and liver/body weight at doses ≥300 ppm. Significantly increased liver/body weight ratios were observed at doses ≥2000 ppm. Significant decreases in kidney/body weight ratio were observed at ≥300 ppm, but the effect was not dose dependent. Body weights were increased at 10,000 ppm and brain/body weight ratios were decreased at 300 and 10,000 ppm. Hypertrophy and/or cytoplasmic vacuolization of hepatocytes were observed at ≥2000 ppm in M and ≥300 ppm in F. The NOEL was 50 ppm. [Note: PBA (2001) states "A statistically significant increase in mean liver weight, in liver to body and/or liver to brain ratios was observed in males and females from group 5 (10,000 ppm) and 4 (2,000 ppm), and in females in group 3 (300 ppm)." However, data provided do not separate effects by sexes.]	PBA (2001); U.S. EPA (2010r)

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
tBuPrAcid-BZT	84268-36-0	Rat, albino RAI, age n.p., 5M/dose	Orally gavaged with 10, 50, and 200 mg/kg for 14 days	No toxicity was observed during treatment. Decreased body weight observed at ≥50 mg/kg with the decrease at the highest dose being significant. Increase in absolute liver weight observed at all doses. Increased microsomal cytochrome P450 content, microsomal epoxide hydrolase activity, and peroxisomal fatty acid β-oxidation activity, and decreased UDP-glucuronosyl-transferase activity and glutathione *S*-transferase activity were observed. Immunoblot analyses showed an increase in cytochrome P452 content, but not Phenobarbital-inducible P450 isozymes b and e. Morphological evaluations of hepatocytes showed increased peroxisome proliferation and "marginal proliferation of smooth endoplasmic reticulum."	Ciba-Geigy (1992b); Thomas et al. (1995)
tBuPrMeEst-BZT	84268-33-7	Rat, albino RAI, age n.p., 5M/dose	Orally gavaged with 10, 50, and 200 mg/kg for 14 days	Increase in absolute liver weight observed. Increased microsomal cytochrome P450 content, microsomal epoxide hydrolase activity, and peroxisomal fatty acid β-oxidation activity, and decreased UDP-glucuronosyl-transferase activity and glutathione *S*-transferase activity were observed. A non-dose dependent increase in ethoxycourmarin *O*-de-ethylase was also observed (at 50 mg/kg). Immunoblot analyses showed an increase in cytochrome P452 content but not phenobarbital-inducible P450 isozymes b and e. Morphological evaluations of hepatocytes showed increased peroxisome proliferation.	Ciba-Geigy (1992b); Thomas et al. (1995)

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
tBuPrMeEst-BZT	84268-33-7	Rat, RAIf, ~6 weeks, 5M&5F/dose	Orally gavaged with 50, 200, and 1000 mg/kg for 29 days	Body weight gain was only decreased in 1000 mg/kg M. No deaths were observed and limited clinical signs of toxicity were seen. Plasma alanine aminotransferase activity was increased in both sexes at the high dose. Aspartate aminotransferase activity was increased in M at 1000 mg/kg and in F at 200 and 1000 mg/kg. Increased plasma urea and bilirubin and decreased plasma globulin were noted in high-dose M. Increased absolute and relative liver weights were observed in all M rats. Increased liver weight was observed in F dosed with 200 and 1000 mg/kg. Absolute and relative kidney weights were increased in F only (≥200 mg/kg). Enlarged livers were only seen in M. Diffuse hepatocyte hypertrophy was noted in both sexes, while liver necrosis was only seen in M. The NOEL was <50 mg/kg.	Ciba-Geigy (1986b)
tBuPrHexEst-BZT	84268-08-6	Rat, strain, age, and number n.p., M	Orally gavaged with 2, 12, 100, and 650 mg/kg for 13 weeks	Increase in absolute liver weight observed. Increased microsomal cytochrome P450 content and peroxisomal fatty acid β-oxidation activity, and decreased UDP-glucuronosyl-transferase activity were observed. Ethoxycoumarin *O*-de-ethylase activity was increased at 50 and 100 mg/kg while glutathione *S*-transferase activity was decreased at 100 mg/kg.	Thomas et al. (1995)

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
mPEG/dPEG (Tinuvin 1130*)	104810-48-2/104810-47-1	Rat, tif: RAIf, age n.p., 24 M/dose	Orally gavaged with 2, 50, and 100 mg/kg for 114 days	Increase in absolute liver weight observed. No effect on microsomal protein content was noted, while a dose-dependent decrease in cytosolic protein content was observed. Decreased microsomal hydrolase activity and glutathione *S*-transferase activity were observed at 50 and 100 mg/kg. Comparatively, increased peroxyiomal fatty acid β-oxidation activity and bilirubin UDP-glucuronosyltransferase activity were observed at all tested doses. Dose-dependent increases in lauric acid 11- and 12-hydroxylase activity and decreases in morphine UDP-glucuronosyltransferase activity were noted. Ethoxyresorufin *O*-de-ethylase activity was significantly decreased at 100 mg/kg and pentoxyresorufin *O*-depentylase was increased at 50 mg/kg. Immunohistochemical studies indicated conflicting effects on various microsomal P450 isoform levels. Total number and structural changes were increased in hepatocyte organelles. Enlarged hepatic peroxisomes containing matrical plates were observed at 50 and 100 mg/kg.	Ciba-Geigy (1992c); Thomas et al. (1995)
Tinuvin 1130†		Rat, Crl CD Br, ~6 weeks, 5M&F/dose	Oral treatment with 10, 50, 200, and 1000 mg/kg for 28 days	No clinical signs were observed at 10 mg/kg/day for F and at 10 and 50 mg/kg/day for M. Drooling was observed in M and F at 200 and 1000 mg/kg. Alopecia was observed in F at 50 and 1000 mg/kg. 4/5 M died at the highest dose. At 10, 200, and 100 mg/kg, one F died in each group. Decreased body weights were seen at 200 and 1000 mg/kg and 1000 mg/kg in M and F, respectively. Increased albumin levels were noted in all dosed F and 50 and 200 mg/kg M. β-Globulin levels were decreased in 200 mg/kg M and 200 and 1000 mg/kg F. Increased patelet counts in M and F at ≥200 mg/kg and decreasedin lymphocytes in three animals at 1000 mg/kg were noted. Increased alkaline phosphatase activity was observed in M and F at 200 mg/kg and F at 1000 mg/kg. Reduced organ size and weight changes were observed in M and F at 200 and/or 1000 mg/kg. A dose-dependent increase in the development of liver necrosis foci was observed starting at 50 mg/kg. Renal tubular degeneration was noted in all M at 1000 mg/kg.	Ciba-Geigy (1986c)

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
Tinuvin 1130*		Rat, Tif: RAI f, min. 6-7 weeks, 25 M&F/dose	Orally gavaged 2, 50, and 100 mg/kg for 70 days prior to and through mating for M and 14 days prior through mating, gestation, and lactation for F	Altered body weight gains were observed in M and F at 50 and 100 mg/kg. Enlarged liver was noted in M at 50 and 100 mg/kg. Increased liver weight and liver to body weight ratios were noted in both sexes at 50 and 100 mg/kg. Hepatocyte hypertrophy was noted in both sexes at the same doses. Hepatocyte necrosis or multifocal organizing necrosis of the liver parenchyma was also noted. Increased mean kidney weight and kidney to body weight ratios were noted in M at 50 and 100 mg/kg and F at 100 mg/kg.	Ciba-Geigy Corporation (1991)
Tinuvin 1130°		Rat, Sprague-Dawley Crl CD (SD) BR, age n.p., 10-20 M&F/dose	Orally gavaged 2, 5, 10, and 50 mg/kg for 91 days, subset allowed to recover prior to euthanization	Body weight gain in high-dose M was decreased compared to control. No clinical signs of toxicity or treatment-related deaths were noted. Blood chemistry changes (e.g., lower packed cell volume) were not considered to be toxicologically significant or treatment related in the report. Increase absolute and relative liver weights were noted in both sexes at all doses. Microscopic liver findings included congestion, granulomas, and vacuoles. Decreased absolute adrenal weight and increased relative kidney and testes weights were noted in high dose M. Gross liver effects reversed after the recovery period. The NOAEL was 10 mg/kg.	Ciba-Geigy Corporation (1992d)

Abbreviations: F = female(s); M = male(s); NOAEL = no observed adverse effect level; NOEL = no observed effect level; n.p. = not provided; TD_{Lo} = lowest toxic dose; UDP = uridine-5'-diphosphate

*The chemical tested in the report was identified as a reaction product between β-[3-(2H-benzotriazol-2-yl)-4-hydroxy-5-*tert*-butylphenyl]propionic acid, methyl ester and polyethylene glycol (identified as Tinuvin 1130). The cover letter noted that the two major chemical components present in the reaction mixture were mPEG and dPEG. However, since all the products were not characterized in the report the product name used in the report has been used.

†The chemical tested was identified as a reaction product between β-[3-(2H-benzotriazol-2-yl)-4-hydroxy-5-*tert*-butylphenyl]propionic acid, methyl ester and polyethylene glycol. Based on other reviewed literature the reaction products are mPEG, dPEG, and propylene glycol. However, since the products were not characterized in the report the product name used in the report has been reported.

°The chemical tested was identified as reaction mixture (Trade names Tinuvin 213 and Tinuvin 1130) typically containing 30-35% dPEG, 50-60% mPEG, and 12-15% propylene glycol.

9.1.5 Chronic Exposure

Chronic exposure studies were identified for only two chemicals, drometrizole and ditBu-BZT. Liver effects were noted in animals after treatment with both chemicals. Increased liver weights in the absence of gross or microscopic changes were noted in mice after treatment with drometrizole for two years. A similar effect in rats treated with drometrizole was not noted. Enlarged livers accompanied by histopathological changes were observed in rats treated with ditBu-BZT for 52 weeks. Hematological effects and increased relative organ weights (e.g., brain and testes) were also observed after ditBu-BZT treatment at the highest dose.

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
Drometrizole	2440-22-4	Mouse, Tif:MAGF (SPF), ~4 weeks old, 50/sex/dose; M&F	5, 50, or 500 ppm in food for 24 months	No effects on body weight gain, food consumption, and survival time were noted in M or F. No signs of toxicity were observed. Decreased liver weights were noted in M administered 50 ppm. Slight increase in adrenal weights was noted in all treated F. No gross or microscopic changes associated with treatment were observed.	U.S. EPA (2010o)
		Rat, CFY, 24-26 days old, 50/sex/dose, M&F	100, 300, 1000, or 3000 ppm in food for 104 weeks	Survival rates were not significantly different from control animals. Decreased body weight gain was observed in 3000-ppm M during the last 52 weeks of treatment. Reduced food intake was also noted among F at the highest dose level from treatment weeks 53 to 80. At the highest dose, an increase in blood nitrogen levels was noted in M at 26 and 102 weeks. Histopathological evaluations did not show any abnormalities associated with treatment. The NOEL was 1000 ppm.	CIR Expert Panel (2008 [PMID:18569163]); U.S. EPA (2010o)

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
ditBu-BZT	3846-71-7	Rat, Crl:CD(SD) IGS, 5 weeks old (6 weeks old at treatment), 20/sex/dose, M&F	M orally gavaged with 0.1, 0.5, or 2.5 mg/kg and F with 0.5, 2.5, or 12.5 mg/kg for 52 weeks	Two M given 0.1 mg/kg were found dead on days 231 and 357. No treatment-related clinical signs of toxicity were noted. However, body weight was decreased from day 36 to the end of the dosing period in high-dose M. Increased in food consumption was observed on days 120, 204-288, and 364 in M. Osmotic pressure was increased in M at doses ≥0.5 mg/kg and decreased in high-dose F. Urine volume was increased in high-dose F. Hematological effects were noted at doses ≥0.5 and 12.5 mg/kg in M and F, respectively. Enlarged livers, increased absolute liver weight, and increased relative liver weight were noted at ≥0.5 and 12.5 mg/kg in M and F, respectively. Histopathological changes in the liver (i.e., centrilobular hypertrophy of hepatocytes with eosinophilic granular cytoplasm, altered hepatocellular foci, and lipofuscin deposition) were also observed. Increased relative brain, pituitary, thyroids, lungs, heart, kidneys, testes, and epididymides weights were noted in high-dose M.	Hirata-Koizumi et al. (2008d [PMID:18161509])

Abbreviations: F = female(s); M = male(s); NOAEL = no observed adverse effect level; NOEL = no observed effect level; n.p. = not provided

9.1.6 Synergistic/Antagonistic Effects

No data were located.

9.1.7 Cytotoxicity

At a concentration of 13 µM (high possible concentration soluble in 0.1% ethanol), drometrizole inhibited concanavalin A-stimulated rat spleen cell proliferation by 6% (Aronsson et al., 2000 [PMID:11074423]).

tBuPrAcid-BZT was cytotoxic to rat and guinea pig hepatocytes as concentrations >10 µM (Ciba-Geigy, 1992e).

9.2 Reproductive and Teratological Effects

The chemicals tested produced a variety of effects. Two of the tested compounds (i.e., drometrizole and ditBu-ClBZT) did not have any effects on reproduction indices (e.g., mating ratio or preimplantation loss). While drometrizole did not affect pup development, ditBu-ClBZT exposure was shown to decrease pup body weight and increase liver weight. diMeEtPh-BZT exposure was associated with a non-dose-dependent decrease in fetal body weight and increase in skeletal maturation delay. Dam and fetal liver effects were noted after exposure to mPEG/dPEG. Additionally, muscular hemorrhages were observed. Some chemicals were shown to affect reproductive organ weights (e.g., ditBu-BZT), but no direct studies in reproduction and development were located. Reproductive and teratological effects after administration of Tinuvin 1130 suggested an association between dosing time and effect. When dams were treated during gestation (days 6-15), minimal effects were noted. Comparatively, when rats were treated prior and during mating and during lactation, effects in reproductive parameters (e.g., number of live births) and pups (e.g., decreased pup weight) were seen.

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
Drometrizole	2440-22-4	Mouse, NMRI, age and number n.p., F	Orally gavaged with 150, 500, or 1000 mg/kg/day on GD 6-15; dams killed on GD 18	No maternal toxicity or embryolethality was noted. No effects on implantation were observed. The compound was not teratogenic. The NOEL was 1000 mg/kg.	U.S. EPA (2010o)
		Mice, NMRI albino, age n.p., 20M/dose	Orally gavaged with 1000 or 3000 mg/kg/day; each M then placed in cage with 2 untreated F and another 2 F after 1 week. F were necropsied on GD 14.	No effects on mating ratio, number of implantations, or embryonic deaths were noted.	U.S. EPA (2010o)
		Rat, Sprague-Dawley, age and number n.p., F	Orally gavaged with 150, 500, or 1000 mg/kg/day on GD 6-15; dams killed on GD 21	No maternal toxicity or embryolethality were noted. No effects on implantation were observed. The compound was not teratogenic. The NOEL was 1000 mg/kg.	U.S. EPA (2010o)
ditBu-BZT	3846-71-7	n.p.	n.p.	Chronic Toxicity study notes increased testes and epididymides weights in high-dose M rats (Hirata-Koizumi et al., 2008d [PMID:18161509]).	

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
ditBu-ClBZT	3864-99-1	Rat, Crj:CD(SD)IGS, 11 weeks old (M) and 10 weeks old (F), 10 or 15/sex/dose, M&F	Orally gavaged with 2.5, 25, or 250 mg/kg starting 28 days prior to mating: M were dosed for 56-57 days and F were dosed 55-69 days (through lactation day 3). M euthanized on day 56-57 and F either euthanized on days 4-6 after parturition or were kept for an additional 14-day recovery period.	No deaths were noted in M or F. No effects on body weight, food consumption, or general condition were observed. There were no effects on the copulation index, fertility index, gestation index, precoital interval, gestation length, numbers of corpora lutea or implantations, preimplantation loss, numbers of pups delivered, live pups, stillborn or sex ratio of live pups, or viability or body weight of pups. No treatment-related morphological anomalies were noted in the pups.	Ema et al. (2008 [PMID:18622873])
		Rat, Crj:CD(SD)IGS, 11 weeks old (M) and 10 weeks old (F), number n.p., M&F F rats were mated with M rats overnight. Copulated F rats were divided into 10/group.	Orally gavaged with 62.5, 250, or 1000 mg/kg/day on GD 5-19	Maternal toxicity was not observed. No effects were noted on ovarian or gravid uterine weight, fertility rate, body weight gain, or feed consumption. There were also no significant effects in the number of corpora lutea, implantations, live fetuses, resorptions/dead fetuses, incidence of pre- or postimplantation embryonic loss, viability of fetuses, fetal weight, or sex ratio of live fetuses. Additionally, no alterations in the incidence of fetuses with malformations or variations or degree of ossification were noted.	Ema et al. (2006 [PMID:16707329])
		Rat, Crj:CD(SD), newborn, 4/sex/dose (littermate), M&F	Orally gavaged with 250 or 500 mg/kg/day on postnatal days 4-21; necropsied on postnatal day 22	In newborn rats (both sexes), a decrease in body weight and increases in absolute and relative liver weights and levels of aspartate aminotransferase, alanine aminotransferase, alkaline phosphatase, and total bilirubin in plasma were seen. Livers showed unspecified histopathological changes. [Note: The abstract states that rats were given the compound on postnatal days 4-21 and newborns were necropised on day 22. Results are then presented for dams and newborn pups. It is unclear from the abstract if dams were administered the same doses or if the results presented are from a previous study.]	Ema et al. (2006 abstr.)

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
ditPe-BZT	25973-55-1	n.p.	n.p.	Subchronic Toxicity study notes increased testes weights in M rats (U.S. EPA, 2010q). [Note: Another source stated "No effects on reproductive organs in Repeat dose testing" (U.S. EPA, 2004).]	
diMeEtPh-BZT	70321-86-7	Rat, Tif:RAIF (SPF) albino, ~2 months old, number n.p., F	300, 1000, or 3000 mg/kg on GD 6-15; dams killed prior delivery	No effects on maternal body weight gain or food consumption were observed. No clinical signs of toxicity noted. No effect on embryo- or fetal-lethality was observed. Group mean fetal body weights were decreased only at 1000 mg/kg dose. Increased delay of skeletal maturation was noted at 1000 mg/kg.	U.S. EPA (2010r)

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
mPEG/dPEG	104810-48-2/104810-47-1	Rat, species and age, and number not provided, 6 dams, F	Single daily dose of 150 mg/kg on GD 6-14, 6-17, or 6-20. Foetuses examined on GD 18 or 21.	Dam livers showed "moderate to striking peroxisome proliferation at all investigated periods of gestation." Peroxisomes were identified as "slightly increased" or "increased." No mitochondrial changes and a slight decrease in glycogen content on GD 21 were noted. Absolute liver weight was increased. Additionally, peroxisomal fatty acid β-oxidation, lauric acid 11- and 12-hydroxylase, and catalase activities were increased at all time points. Liver malondialdehyde content was increased at GD 15. Selenium-dependent and -independent glutathione peroxidase activities were decreased at GD 15, 18, and 21, and 21, respectively. Subcutaneous and skeletal muscular hemorrhages within the connective tissues noted. Peroxisome proliferation was moderately to strikingly increased at all time points in fetuses. Peroxisome size was also increased. Increased mitochondrial volume and enlarged mitochondria were noted on GD 18 and 21. Glycogen content was "marginal" on GD 18 and 21. Absolute liver weight was not affected. Peroxisomal fatty acid β-oxidation activity was increased at all time points while lauric acid 11- and 12-hydroxylase, and catalase activities were increased at GD 18 and 21. Liver malondialdehyde content was increased at GD 21. Liver total glutathione content and liver content of reduced glutathione were decreased on GD 21 while selenium-dependent glutathione peroxidase activity was increased on GD 21.	Thomas et al. (1995)

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
Tinuvin 1130*		Rat, Tif: RAIf, min. 8 weeks, 24 mated rats/dose	Orally gavaged 1, 30, and 150 mg/kg on GD 6-15. Dams killed on GD 21.	Maternal body weight decreased at the highest dose, with feed consumption reduced at 30 and 150 mg/kg. No treatment-related deaths or clinical signs were observed. No effect was noted on preimplantation loss, number of implantation sites, early and late post-implantation loss, and number of live fetuses/litter. Fetal body weights were not altered at any of the tested doses. Delayed ossification was noted at 150 mg/kg.	Ciba-Geigy (1993)
		Rat, Tif:RAIf, ~2 months old, 8M&F/dose	Orally gavaged 20, 100, and 200 mg/kg for 1 week prior to and through mating for M and 1 week prior through mating and 14 days after birth got F	No dose-related effects on body weight, body weight gain, or food consumption were noted in eother sex at any tested dose. Additionally, no clinical signs of toxicity were noted in any dose group for either sex. Isolated findings were observed during necropsy (e.g., reduced testicle size in 1 M), but no overall test article effects were observed. Decreased weight was observed in the 20 and 200 mg/kg dose groups during lactation. No live births were noted for high dose F; all stillborn pups had dark and necrotic skin on the abdomen and hind limbs. Number of delivered pups and number of live pups was decreased for 200 and 100 mg/kg dose groups, respectively. Prenatal and perinatal loss were increased in both of these dose groups. Mean pup body weight also was decreased for the 100 mg/kg dose. Pups from the 100 mg/kg had necrotic skin on the abdomen and atrophic and necrotic skin on the right hind limb.	Ciba-Geigy (1990)

Chemical	CASRN	Species, Strain, Age, Number, and Sex of Animals	Doses Tested/Route of Administration	Results/Comments	Reference(s)
Tinuvin 1130*		Rat, Tif: RAI f, min. 6-7 weeks, 25 M&F/dose	Orally gavaged 2, 50, and 100 mg/kg for 70 days prior to and through mating for M and 14 days prior through mating, gestation, and lactation for F	Body weight effects noted in M and F. No macroscopic or microscopic effects in reproductive systems noted. No effect on M fertility parameters noted. Reduced live birth index was noted at 50 and 100 mg/kg. Increased prenatal loss and decreased pup survival up to PND 4 were noted at 100 mg/kg. Additionally, reduced birth weight and mean pup weight during lactation, and delayed eye opening and tooth eruption were noted at the highest dose.	Ciba-Geigy (1991)

Abbreviations: F = female(s); GD = gestation day(s); M = male(s); NOEL = no observed effect level; n.p. = not provided

*The chemical tested was identified as a reaction product between β-[3-(2H-benzotriazol-2-yl)-4-hydroxy-5-*tert*-butylphenyl]propionic acid, methyl ester and polyethylene glycol (identified as Tinuvin 1130). The cover letter noted that the two major chemical components present in the reaction mixture were mPEG and dPEG. However, since all the products were not characterized in the report the product name used in the report has been reported.

9.3 Carcinogenicity

Male and female MAGf (SPF) mice were fed 5, 50, or 500 ppm drometrizole in diet daily for 24 months. Benign and malignant tumors were observed in both controls and treated mice but were not considered treatment related (CIR Expert Panel, 2008 [PMID:18569163]). Similarly, tumor formation in CFY male and female rats was not significantly different from controls and the distribution was not affected by treatment with 100, 300, 1000, or 3000 ppm drometrizole for 104 weeks (CIR Expert Panel, 2008 [PMID:18569163]; U.S. EPA, 2010o).

9.4 Initiation/Promotion Studies

No data were located.

9.5 Genotoxicity

None of the tested compounds were identified as mutagenic *in vitro* in the absence or presence of a metabolic system (S9) or *in vivo*.

Chemical	CASRN	Results	Reference(s)
Drometrizole	2440-22-4	Not mutagenic to *Salmonella typhimurium* strains TA98, TA100, TA1535, or TA1537 in the absence or presence of S9. Not mutagenic to *S. typhimurium* strain TA1538 in the presence of S9. *In vivo* studies (e.g., dominant lethal assay in mice and evaluation of micronucleated erythrocytes in mouse bone marrow and chromosomal aberrations in hamster bone marrow) also indicated that drometrizole was not mutagenic.	CIR Expert Panel (2008 [PMID:18569163]); Jonsen et al. (1980)*; U.S. EPA (2010o)
Octrizole	3147-75-9	Not mutagenic to *S. typhimurium* strains TA98, TA100, TA1535, and TA1537 in the absence or presence of S9, or *Escherichia coli* WP2 uvr A in the absence or presence of S9. Octrizole was also not mutagenic in the SOS Chromotest in the absence or presence of S9.	He et al. (2003 [PMID:14680371]); U.S. EPA (2010p)
Bumetrizole	3896-11-5	Not mutagenic to *S. typhimurium* strains TA98 or TA1538 in the presence of S9.	Jonsen et al. (1980)*
ditBu-BZT	3846-71-7	Not mutagenic to *S. typhimurium* [strains not provided] or *E. coli* in the absence or presence of S9. Not mutagenic to *S. typhimurium* strains TA98 or TA1538 in the presence of S9. Did not produce chromosomal aberrations in cultured Chinese hamster lung cells in the absence or presence of S9.	Hirata-Koizumi et al. (2009a [PMID:20021483]); Jonsen et al. (1980)*
ditBu-ClBZT	3864-99-1	Not mutagenic to *S. typhimurium* strains TA98 or TA1538 in the presence of S9.	Jonsen et al. (1980)*
ditPe-BZT	25973-55-1	Not mutagenic in *S. typhimurium* strains TA97, TA98, TA100, or TA102 or *E. coli* strain WP2/pKM101 [Note: No information on use of metabolic activation system was provided in abstract.]. Not mutagenic to *S. typhimurium* strains TA98 or TA1538 in the presence of S9.	Hachiya and Takizawa (1994); Jonsen et al. (1980)*
diMeEtPh-BZT	70321-86-7	Not mutagenic in *S. typhimurium* strains TA98, TA100, TA1535, or TA1537 in the presence of absence of S9. It was negative for the induction of DNA damage using rat hepatocytes. In *in vivo* studies in hamsters, it was negative for chromosomal aberrations and sister chromatid exchange in bone marrow.	U.S. EPA (2010r)

Chemical	CASRN	Results	Reference(s)
Tinuvin 1130†		Not mutagenic in *S. typhimurium* strains TA98, TA100, TA1535, or TA1537 in the presence of absence of S9. In *in vivo* studies in hamsters, the compound was not mutagenic.	Ciba-Geigy Corporation (1987)

*The authors noted that two of the tested chemicals gave conflicting results, which were classified as negative. There is no information as to which two gave conflicting results.
†The composition of the tested substance was not provided.

9.6 Cogenotoxicity

No data were located.

9.7 Immunotoxicity

No data were located.

9.8 Other Data

Chemical	CASRN	Results	Reference(s)
Drometrizole	2440-22-4	Not estrogenic in yeast-two hybrid assay or transiently transfected 293T cells.	Kawamura et al. (2003); Ogawa et al. (2006 [PMID:16546889]); Wada et al. (2004 [PMID:14981123])
		Exhibited minimal agonist activity in yeast two-hybrid estrogenicity assay incorporating medERα in presence of S9 only (EC ×10 = 15 μM); no activity seen in the hERα assay with or without S9. Binding affinity was low; IC_{50} was >37,500 nM in an ER-ELISA with and without S9.	Terasaki et al. (2007 [PMID:17941731])
		Classified as a mild ocular irritant in rabbit eyes (dose = 500 mg)	RTECS (2010)
		Drometrizole was identified as a non-sensitizer in the murine local lymph assay after dermal administration. It also was identified as a non-sensitizer in the Magnusson-Kligman maximization test in guinea pigs. However, it was classified as a sensitizer when initially administered by intradermal injection followed by topical exposure for three days. Drometrizole was also classified as a sensitizer using the mouse ear swelling test where it was administered intradermally followed by topical challenge.	CIR Expert Panel (2008 [PMID:18569163]); Ikarashi et al. (1994a [PMID:8171445], 1994b [PMID:8033549])

Chemical	CASRN	Results	Reference(s)
Octrizole	3147-75-9	Not estrogenic in a yeast estrogen assay or transiently transfected 293T cells. Not classified as an androgen agonist or antagonist in a Chinese hamster ovary cell line stably transfected with rat androgen receptor response element fused to a luciferase gene and an androgen receptor. Identified as inactive in 11 bioassays noted in PubChem, including inhibitors of the interaction of thyroid hormone receptor and steroid receptor coregulator 2, ROR γ transcriptional activity, and Bloom's syndrome helicase.	Miller et al. (2001); Wada et al. (2004 [PMID:14981123]) Araki et al. (2005 [PMID:15950433]) PubChem (undated-b)
Bumetrizole	3896-11-5	Not estrogenic in yeast-two hybrid assay.	Kawamura et al. (2003); Ogawa et al. (2006 [PMID:16546889])
ditBu-ClBZT	3864-99-1	Not estrogenic in yeast-two hybrid assay. Also had no androgenic activity in AR-EcoScreen cells.	Araki et al. (2005 [PMID:15950433]); Kawamura et al. (2003)
ditPe-BZT	25973-55-1	Not estrogenic in yeast-two hybrid assay.	Kawamura et al. (2003); Ogawa et al. (2006 [PMID:16546889])
diMeEtPh-BZT	70321-86-7	Not estrogenic in yeast-two hybrid assay. Predicted to have low relative binding affinity for estrogen receptor using the MultiCASE expert system (Predicted RBA <0.0001; probability the prediction result was correct was 52%)	Kawamura et al. (2003); Klopman and Chakravarti (2003 [PMID:12615097]); Ogawa et al. (2006 [PMID:16546889])
Bisoctrizole	103597-45-1	Did not bind to estrogen or androgen receptors isolated from rat uteri or testes, respectively. Additionally, was inactive in the immature rat uterotrophic assay. *In vitro* and *in vivo* studies were conducted to assess absorption of an emulsion containing bisoctrizole. *In vitro*, 89.4% of the amount recovered in the upper stratum corneum (15 tape strippings) of abdominal skin explants. Bisoctrizole was also found in the epidermal and dermal compartments. Of the total applied dose, 92.2% was obtained in 15 tape strippings *in vivo.*	Ashby et al. (2001 [PMID:11754532]) Mavon et al. (2007 [PMID:17035717])
tBuPrAcid-BZT	84268-36-0	Increased cyanide insensitive β-oxidation of long chain fatty acids in rat, but not guinea pig, hepatocytes. [ILS Note: The report notes that the effect is characteristic of peroxisome proliferators.]	Ciba-Geigy (1992e)

A TSCA submission by Ciba-Geigy evaluated the guinea pig skin sensitization potential of a reaction mixture that typically contained 30-35% dPEG, 50-60% mPEG, and 12-15% polyethylene glycol (trade names Tinuvin 213 and Tinuvin 1130). The mixture induced sensitization in 50-70% of the tested animals (Ciba-Geigy, 1992f).

Tinuvin 1130 was not a rabbit skin or eye irritant at a dose of 0.5 and 0.1 g/animal, respectively. Tinuvin 1130 also was not a skin sensitizer in guinea pigs at a concentration of 10% (Ciba-Geigy Corporation, 1987).

U.S. EPA New Chemicals Program

The New Chemicals Program at the EPA summarized toxicity of the benzotriazole-hindered phenol class. The summary noted that increased organ weights, hematological effects, and immune system effects were associated with this chemical class. Male and female reproductive toxicity were also noted with this class of chemicals. Males appeared to be more sensitive than females. Dermal sensitization was also noted with these chemicals (U.S. EPA, 2010s).

10.0 Structure-Activity Relationships

10.1 Structurally Similar Chemical

Benzotriazole is the core structure present within the phenolic benzotriazole class. *In vitro* metabolism with rat liver microsomes yielded formation of 5- and 4-hydroxybenzotriazole (1.6 and 0.32% of the amount added, respectively). Overall metabolism was low (<5% of the total amount added) (Stouten et al., 2000). Oral acute studies in rats and mice yielded LD_{50} values that ranged from 560 to 909 mg/kg. Intraperitoneal LD_{50} values in mice and rats ranged from 400-1000 and 500-900 mg/kg, respectively. A mouse intravenous LD_{50} of 238 mg/kg was identified. Dermal LD_{50} values were ≥1000 mg/kg in rats and rabbits, and inhalation LC_{50} values in rats were 1.5 mg/L and 1.91 mg/L/3 hours (ChemIDplus, undated; HSDB, 2003; Stouten et al., 2000; U.S. EPA, 2010t). Subcronic and short-term studies showed that oral administration to mice produced minimal effects on body weight while dose-dependent decreases in body weight were observed in rats. Endocrine effects, normocytic anemia, and leukopenia were noted in rats dosed for 26 weeks. The TD_{Lo} was 109 mg/kg (RTECS, 2009; Stouten et al., 2000). No effects on deaths and no clinical symptoms were noted in mice or rats orally administered (in food) benzotriazole ≥78 weeks. Additionally, no dose-related effects on reproductive organs were noted in either sex (U.S. EPA, 2010t). Neoplastic liver nodules were observed in male Fischer rats fed 12,100 ppm benzotriazole for 78 weeks. However, historic laboratory controls incidences varied from 0 to 11% so the treatment-related effects could not be determined. Brain tumors occurred in three males and one female rat. Incidence of endometrial stromal polyps was increased significantly in female rats fed 6700 ppm for 78 weeks (22%), but not in female rats fed 12,100 ppm (16%). Significant increase in alveolar/bronchiolar carcinomas (18%) was observed female B6C3F1 fed 11,700 ppm benzotriazole for 104 weeks. Comparatively, a similar increase was not observed in female mice fed 23,500 ppm benzotriazole for the same period of time (6% increase). Historical laboratory control incidences varied from 0 to 7% (NCI, 1978; U.S. EPA, 2010t). Genotoxicity studies indicate that the compound was not mutagenic to *S. typhimurium* strains TA97, TA98, or TA100 in the presence or absence of S9, or Chinese hamster ovary cells. Benzotriazole was also not mutagenic to *S. typhimurium* strain TA1535 in the absence of S9, but was mutagenic in the presence of S9. Conflicting results were obtained for effects in *S. typhimurium* strains TA1537 and TA1538 and *E. coli* WP2 *uvrA*. It did not produce DNA damage in *E. coli* PQ37. In Chinese hamster ovary cells, benzotriazole induced chromosomal aberrations in the presence of S9 and sister chromatid exchange in the absence of S9. Benzotriazole was not genotoxic in the mouse micronucleus assay at 800 mg/kg (CCRIS, 2003; NTP, undated-a, undated-b, undated-c; Stouten et al., 2000; U.S. EPA, 2010t). Benzotriazole was identified as a non-sensitizer in the guinea pig maximization test (U.S. EPA, 2010t). Benzotriazole was identified as irritating to rabbit eyes and minimally irritatibg to rabbit and guinea pig skin (Stouten et al., 2000).

10.2 Leadscope Structure-Activity Relationship Evaluation

For each Leadscope model suite evaluated, a positive prediction probability (ranging from 0-1) was calculated. Values ≥0.5 were defined as positive. If the test compound was not at least 30% similar to one in the training set and at least one model feature was not in the test compounds, the chemical was defined as "not in the domain" and prediction probability was not determined.

The full list of prediction results is provided in Appendix E. In the following summary, models within each suite of models where seven or greater evaluated chemicals were predicted to be positive are discussed.

<u>Genetic Toxicity</u>

The 29 genetic toxicity models in Leadscope encompass predictions for mutagenicity (13), DNA damage (3), *in vivo* clastogenicity (5), and *in vitro* clastogenicity (8). Sensitivity and specificity of the models range from 6.67% to 96% and 38.7% to 96.8%, respectively. The SCE in vitro CHO and SCE in vitro Other Cell models had ≥7 positive predicted chemicals.

SCE in vitro CHO

The table below provides the predicted probabilities for the model and the percentage contribution of the features and physical-chemical properties evaluated to the calculated prediction value.

	P-BZT	Drometrizole	tBu-BZT	EtOH-BZT	Ethanone-BZT	MaOE-BZT	Allyl-BZT	OcOx-BZT
Positive Prediction Value	0.755	0.66	0.522	0.598	0.633	0.88	0.573	0.697
% Feature contribution	38.56%	32.08%	40.02%	31.0%	34.62%	99.1%	37.89%	107.9%
% Property contribution	61.44%	67.92%	59.98%	69.0%	65.38%	0.8951%	62.11%	-7.875%

The table below lists the structural features identified as contributing to the activity of the noted chemical.

Feature	P-BZT†	Drometrizole†	tBu-BZT†	EtOH-BZT†	Ethanone-BZT†	MaOE-BZT†*	Allyl-BZT†	OcOx-BZT†
aminobenzene	X	X	X	X	X	X	X	X
oxybenzene	X	X	X	X	X	X	X	X
isopropylbenzne			X					
benzene	X	X	X	X	X	X	X	X
ethylbenzene			X	X	X	X	X	
toluene		X	X	X	X	X	X	
hydroxybenzene	X	X	X	X	X	X	X	X
4-methylphenol		X	X		X	X	X	
4-isopropylphenol			X					

Feature	P-BZT†	Drometrizole†	tBu-BZT†	EtOH-BZT†	Ethanone-BZT†	MaOE-BZT†*	Allyl-BZT†	OcOx-BZT†
1-(alkyl, acyc)-benzene		X	X	X		X	X	
propane			X	X	X	X	X	X
alkenyl, acyc carboxylate						X		
alkenyl, acyc-carbonyl						X		
p-anisidine								X
1-methoxypentane								X
pentol								X
hexanol								X
heptanes								X
octane								X
hexane								X
butane								X

†For these chemicals, an oxybenzene moiety was identified twice and a hydroxybenzene moiety was identified once. However, all three entries referred to the same group in the compounds. While the oxybenzene moiety entries were positive associated with activity the hydroxybenzene moiety was negative associated with activity.
*For this chemical, an alkenyl, acyc carboxylate/alkenyl-carboxylate moiety was identified three times as a contributing structural feature. However, the contribution of the moiety was the same for two entries (25.4%) and greater in the third entry (39.69%).

For most of the chemicals evaluated, the moieties associated with activity were benzene or benzene substituted derivatives. Alkyl chains were also identified as impacting the predicted activity for OcOx-BZT.

The number of structurally similar chemicals for the positive compounds ranged from one to fourteen; these are provided in the table below.

Structurally Similar Chemical	P-BZT	Drometrizole	tBu-BZT	EtOH-BZT	Ethanone-BZT	MaOE-BZT	Allyl-BZT	OcOx-BZT
3,5-di-tert-butyl-4-hydroxytoluene	X	X	X				X	
2-methylphenol	X	X	X				X	
phenol	X	X	X					
hexylresorcinol	X	X	X	X			X	X
bisphenol A	X	X	X					
2-phenylphenol	X	X	X					
1-phenylazo-2-naphthol	X	X	X					
N-(4-((2-hydroxy-5-methylphenyl)azo)phenyl)acetamide		X						
hydroquinone	X	X	X					

Structurally Similar Chemical	P-BZT	Drometrizole	tBu-BZT	EtOH-BZT	Ethanone-BZT	MaOE-BZT	Allyl-BZT	OcOx-BZT
1-((4-methyl-2-nitrophenyl)azo)-2-naphthalenol		X						
2,2',4,4'-tetrahydroxybenzophenone					X			
oxybenzone					X			X
vanillin					X			X
resorcinol	X		X					X
diethylstilbestrol	X							
4-nitrophenol	X							X
oxyquinoline	X							
anthralin	X							X
benzotriazole	X							
diglycidyl resorcinol ether								X
eugenol							X	X
2,4,6-nitrophenol								X
methacrylic acid, ethyl ester						X		
santonox			X					

SCE in vitro Other Cells

The table below provides the predicted probabilities for the model and the percentage contribution of the features and physical-chemical properties evaluated to the calculated prediction value.

	P-BZT	Drometrizole	Ethanone-BZT	Allyl-BZT	Bumetrizole	ditBu-ClBZT	OcOx-BZT
Positive Prediction Value	0.969	0.541	0.955	0.515	0.561	0.508	0.972
% Feature contribution	48.35%	-29.26%	63.28%	-11.51%	30.01%	25.06%	66.34%
% Property contribution	51.65%	129.3%	36.72%	111.5%	69.99%	74.94%	33.66%

The table below lists the structural features identified as contributing to the activity of the noted chemical.

Feature	P-BZT	Drometrizole	Ethanone-BZT	Allyl-BZT	Bumetrizole	ditBu-ClBZT	OcOx-BZT
aminobenzene	X	X	X	X	X	X	X
oxybenzene	X	X	X	X	X	X	X
isopropylbenzne					X	X	

Feature	P-BZT	Drometrizole	Ethanone-BZT	Allyl-BZT	Bumetrizole	ditBu-ClBZT	OcOx-BZT
benzene	X	X	X	X	X	X	X
ethylbenzene			X	X	X	X	
toluene		X	X	X	X	X	
4-methylphenol		X	X	X	X	X	
1-(alkyl, acyc)-benzene		X		X	X	X	
alkenyl, acyc-carbonyl			X				
1-alkyl-4-hydroxy		X		X	X	X	
propane			X	X	X	X	X
4-ethylphenol			X			X	
chlorobenzene					X	X	
phenylhalide					X	X	
alkoxybenzene							X

For most of the chemicals evaluated, the amino- and oxy-benzene moieties were associated with the predicted activity. For those chemicals where a halide was present (e.g., bumetrizole), that moiety had a greater influence on the predicted activity than the benzene-substituted moieties.

The number of structurally similar chemicals for the positive compounds ranged from one to nine; these are provided in the table below.

Structurally Similar Chemical	P-BZT	Drometrizole	Ethanone-BZT	Allyl-BZT	Bumetrizole	ditBu-ClBZT	OcOx-BZT
phenol	X	X					
2-methylphenol	X	X		X	X	X	
LS-105088*	X						
catechol	X						
hydroquinone	X						
resorcinol	X	X					X
diethylstilbestrol	X						
oxyquinoline	X						
guaiacol	X	X					X
vanillin			X				X
isoeugenol							X

*The structure of the structurally similar chemical is unclear, therefore the common and/or scientific name were not sought.

<u>Neurotoxicity</u>

The neurotoxicity models in Leadscope encompass predictions for newborn rat, rodent, and mouse behavior; sub-models represent optimized active/inactive chemicals. Sensitivity and specificity of the models range from 43.2% to 78.4% and 86.4% to 91.4%, respectively. Within this suite, the percentage of chemicals with a positive prediction value versus the total number of chemical that were identified within the scope of the model ranged from 0 to 39%. The Pup Rodent Behavior model was the only model with ≥7 chemicals predicted to be positive.

The table below provides the predicted probabilities for the overall model and the two sub-models. The percentage contribution of the features and physical-chemical properties evaluated, for the overall model, to the calculated prediction value are also provided.

Positive Prediction Value	P-BZT	tBu-BZT	tBu-ClBZT	sButBu-BZT	Bumetrizole	ditBu-BZT	ditBu-ClBZT	tBuPrOCEst-ClBzt
Overall	0.501*	0.6355	0.6155	0.627	0.5125	0.5915	0.56	0.514*
Sub-model A	n.p.	0.418	0.4	0.405	0.293	0.366	0.335	n.p.
Sub-model B	n.p.	0.853	0.831	0.849	0.732	0.817	0.785	n.p.
% Feature contribution	10.79%	36.62%	38.9%	50.32%	28.95%	40.16%	43.73%	124.4%
% Property contribution	89.21%	63.38%	61.1%	49.68%	71.05%	59.84%	56.27%	-24.42%

Abbreviation: n.p. = not provided

*These chemicals were identified as not in domain for one of the sub-models evaluated. However, the current output from Leadscope does not identify which sub-model the results are presented for. Therefore, these results were placed in the overall field. When the output is revised to identify the appropriate sub-model, the table will be revised accordingly.

The table below lists the structural features identified as contributing to the activity of the noted chemical. [ILS Note: Since the endpoint is composed two sub-models, the structural features identified in the overall model are provided below.]

Feature	P-BZT	tBu-BZT	tBu-ClBZT	sButBu-BZT	Bumetrizole*	ditBu-BZT	ditBu-ClBZT	tBuPrOCEst-ClBzt
t-butylbenzene		X	X	X	X	X	X	X
oxybenzene	X	X	X	X	X	X	X	X
toluene		X	X	X	X	X	X	X
phenyl-halide			X		X		X	X
butane				X				X
alkyl, acyc, carbonyl								X
oxycarbonyl, O-alkyl								X
oxycarbonyl, O-(alkyl, acyc)-								X

*For this chemical, a toluene moiety was identified twice as a contributing structural element. In one entry, the moiety was positively associated with activity while another entry indicates that it was negatively associated with activity. Similar differences are observed with both sub-models.

For the seven chemicals that contained a *t*-butyl moiety, this structural feature was the greatest structural feature contributing to the predicted activity for all the chemicals. The oxybenzene, toluene, butane or phenyl-halide moieties also positively contributed to the predicted activity. Comparatively, addition of a carbonyl or ester moiety (as observed in tBuPrOCEst-ClBzt) negatively contributed to the overall prediction value. Of the physical-chemical properties evaluated, the presence of hydrogen bond acceptors was one of the greatest positive contributor to the predicted activity for all the positively predicted compounds.

The number of structurally similar chemicals for the positive compounds ranged from one to four; these are provided in the table below.

Structurally Similar Chemical	P-BZT	tBu-BZT	tBu-ClBZT	sButBu-BZT	Bumetrizole	ditBu-BZT	ditBu-ClBZT	tBuPrOCEst-ClBzt
p-chlorophenol	X		X		X		X	X
penta-chlorophenol			X		X		X	
3-*tert*-butyl-4-methoxyphenol		X	X			X		
2-*tert*-butyl-4-methoxyphenol		X	X	X		X		

<u>Reproductive and Developmental Toxicity</u>

The developmental toxicity models in Leadscope encompass predictions for structural dysmorphogenesis, visceral organ toxicity, fetal survival, and fetal growth. The reproductive toxicity models encompass predictions for toxicity in male and female rats, mice, and rodents. Sub-models in the reproductive and developmental toxicity evaluations represent optimized active/inactive chemical ratios. Sensitivity and specificity of the reproductive models range from 36.3% to 63.8% and 83.9% to 96.5%, respectively. Sensitivity and specificity of the developmental toxicity models range from 22.1% to 57.4% and 84.4% to 95.3%.

<u>Developmental Suite</u>

Within the developmental suite of models, the percentage of chemicals with a positive prediction value versus the total number of chemical that were identified within the scope of the model ranged from 0 to 33%. The Structural Rabbit model was the only model with ≥7 chemicals predicted to be positive.

The table below provides the predicted probabilities for the overall model and the three sub-models. The percentage contribution of the features and physical-chemical properties evaluated, for the overall model, to the calculated prediction value are also provided.

Positive Prediction Value	DoM-BZT	sButBu-BZT	ditBu-BZT	ditPe-BZT	ditOc-BZT	MeEtMeBu-CF_3BZT*	tBuPrAcid-BZT
Overall	0.5227	0.5843	0.601	0.5677	0.5427	0.5545	0.769
Sub-model A	0.598	0.652	0.656	0.637	0.605	0.747	0.885
Sub-model B	0.455	0.523	0.566	0.498	0.472	0.362	0.844
Sub-model C	0.515	0.578	0.581	0.568	0.551	not provided	0.578
% Feature contribution	104.2%	89.97%	88.29%	95.33%	102.2%	102.1%	92.38%
% Property contribution	-4.2%	10.03%	11.71%	4.674%	-2.206%	-2.137%	7.625%

*The prediction value was not calculated for sub-model C. Based on personal communications with Leadscope, this is due to the fact that the chemical was classified as not in domain for that particular sub-model. Therefore, the overall model is only based on the results from sub-models A and B.

The table below lists the structural features identified as contributing to the activity of the noted chemical. [ILS Note: Since the endpoint is composed three sub-models, the structural features identified in the overall model are provided below.]

Feature	DoM-BZT	sButBu-BZT	ditBu-BZT	ditPe-BZT	ditOc-BZT	MeEtMeBu-CF_3BZT	tBuPrAcid-BZT
1-alkyl-4-hydroxybenzene	X	X	X	X	X	X	X
hydroxybenzene	X	X	X	X	X	X	X
1-alkyl-2-hydroxybenzene	X	X	X	X	X	X	X
oxybenzene	X	X	X	X	X	X	X
1,3-dialkylbenzene	X	X	X	X	X	X	X
1,3-dimethylbenzene	X	X	X	X	X	X	X
toluene	X	X	X	X	X	X	X
benzene	X	X	X	X	X	X	X
ethylbenzene	X	X	X	X	X	X	X
1-(alkyl,acyc)-benzene	X	X	X	X	X	X	X
butane	X	X		X	X	X	X
1-hydroxy-4-(3-oxopropyl)benzene							X
alkyl, acyc-carbonyl							X
alkyl-carboxylic acid							X
carboxylic acid							X
propylcarbonyl							X
hexane	X						
trifluormethyl						X	
1-benzyl benzene						X	
monosubstituted benzene						X	

For six of the chemicals, the hydroxybenzene and oxybenzene moieties were identified as the structural features contributing the greatest amount to the predicted activities. The only chemical where this was not the case was MeEtMeBu-CF_3BZT, where the trifluoromethyl was the greatest contributor to the activity. This was closely followed by the hydroxybenzene and oxybenzene moieties. Overall, the carbonyl containing moieties, straight-chained alkyl moieties, benzene substituted compounds were negatively associated with the predicted activity. Of the physical-chemical properties evaluated, the presence of hydrogen bond acceptors was a large contributor to the predicted effect.

The number of structurally similar chemicals for the positive compounds ranged from two to seven; these are provided in the table below.

Structurally similar chemical	DoM-BZT	sButBu-BZT	ditBu-BZT	ditPe-BZT	ditOc-BZT	MeEtMeBu-CF_3BZT	tBuPrAcid-BZT
bisphenol A	X	X	X	X	X	X	
naphthalene-2-ol	X	X	X	X	X		
probucol	X	X	X	X	X		
benzene-1,4-diol			X	X	X		
2-*tert*-butyl-4-methoxyphenol		X	X	X	X		
naphthalene-2,3-diol			X	X	X		
3-*tert*-butyl-4-methoxyphenol			X				
2-(butan-2-yl)-4,6-dinitrophenol		X					
3-(3,4-dimethylphenyl)-2-hydrazinyl-2-methylpropanoic acid							X
2-amino-3-(4-methylphenyl)propanoic acid							X
oxaprozin							X
2-{3-bis(propan-2-yl)amino-1-phenylpropyl}-4-methylphenol	X					X	

__Reproductive Suite__

Within the reproductive models, there were two models where ≥7 tested chemicals were predicted to be positive, repo rat male (7 predicted positive) and repo rat female (10 predicted positive). There were five chemicals that were predicted to be positive in both models. For four of the five common chemicals, the positive prediction value was greater for the repo rat male model when compared to the female model.

Repo Rat Male

The table below provides the predicted probabilities for the model and the percentage contribution of the features and physical-chemical properties evaluated to the calculated prediction value.

	sButBu-BZT	Bumetrizole	ditBu-BZT	ditBu-ClBZT	ditPe-BZT	ditOc-BZT	tBuPrAcid-BZT
Positive Prediction Value	0.715	0.537	0.718	0.57	0.745	0.721	0.691
% Feature contribution	71.12%	84.34%	70.69%	77.11%	66.9%	69.41%	75.29%
% Property contribution	28.88%	15.66%	29.31%	22.89%	33.1%	30.59%	24.71%

The table below lists the structural features identified as contributing to the activity of the noted chemical.

Feature	sButBu-BZT	Bumetrizole	ditBu-BZT	ditBu-ClBZT	ditPe-BZT	ditOc-BZT	tBuPrAcid-BZT
1-alkyl-2-hydroxy-benzene	X	X	X	X	X	X	X
oxybenzene	X	X	X	X	X	X	X
1-(alkyl, acyc)-benzene	X	X	X	X	X	X	X
propane	X	X	X	X	X	X	X
alkyl-carboxylic acid							X
toluene	X	X	X	X	X	X	X
carboxy							X
chlrorobenzene		X		X			
phenyl-halide		X		X			

Except for the chlorobenzene and phenyl halide moieties identified in ditBu-ClBZT and bumetrizole, all the remaining identified structural features were predicted to positively contribute to the predicted activity.

The number of structurally similar chemicals for the positive compounds ranged from one to two; these are provided in the table below.

Structurally Similar Chemical	sButBu-BZT	Bumetrizole	ditBu-BZT	ditBu-ClBZT	ditPe-BZT	ditOc-BZT	tBuPrAcid-BZT
4-[4-(4-hydroxyphenyl)hexan-3-yl]phenol	X		X		X	X	
benzene-1,4-diol			X		X	X	
pentachlorophenol		X		X			

Structurally Similar Chemical	sButBu-BZT	Bumetrizole	ditBu-BZT	ditBu-ClBZT	ditPe-BZT	ditOc-BZT	tBuPrAcid-BZT
2-(butan-2-yl)-4,6-dinitrophenol	X						
2-amino-3-(4-hydroxyphenyl)2-methylpropanoic acid							X
oxaprozin							X

Repo Rat Female

The table below provides the predicted probabilities for the overall model and the four sub-models. The percentage contribution of the features and physical-chemical properties evaluated, for the overall model, are also provided.

Positive Prediction Value	Ethanone-BZT	sButBu-BZT	ditBu-BZT	ditPe-BZT	ditOc-BZT	MeEtPhMeBu-BZT	diMeEtPh-BZT	tBuPrAcid-BZT	Bisoctrizole	Oc-NTZ
Overall	0.792*	0.5098	0.5092	0.5355	0.5615	0.5865	0.518†	0.7682	0.586†	0.5092
Sub-model A	n.p.	0.673	0.672	0.715	0.746	0.85	n.p.	0.965	n.p.	0.581
Sub-model B	n.p.	0.482	0.483	0.484	0.495	0.495	n.p.	0.868	n.p.	0.492
Sub-model C	n.p.	0.428	0.429	0.458	0.481	0.48	n.p.	0.812	n.p.	0.469
Sub-model D	n.p.	0.456	0.453	0.485	0.524	0.521	0.518	0.428	0.586	0.495
% Feature contribution	77.1%	77.16%	77.28%	71.28%	65.92%	68.26%	56.12%	90.17%	46.04%	66.57%
% Property contribution	22.9%	22.84%	22.72%	28.72%	34.08%	31.74%	43.88%	9.831%	53.96%	33.43%

Abbreviation: n.p. = not provided

*This chemical was identified as not in domain for one of the sub-models evaluated. However, the current output from Leadscope does not identify which sub-model the results are presented for. Therefore, these results were placed in the overall field. When the output is revised to identify the appropriate sub-model, the table will be revised accordingly.

†These chemicals were identified as not in domain for at least one of the submodels. Based on the number of chemicals present in the submodel, it was deduced that the results were associated with Sub-model D.

The table below lists the structural features identified as contributing to the activity of the noted chemical and the percentage. [ILS Note: Since the endpoint is composed four sub-models, the structural features identified in the overall model are provided below.]

Feature	Ethanone-BZT	sButBu-BZT	ditBu-BZT	ditPe-BZT	ditOc-BZT	MeEtPhMeBu-BZT	diMeEtPh-BZT	tBuPrAcid-BZT	Bisoctrizole	Oc-NTZ
1-alkyl-4-hydroxy benzene		X	X	X	X	X	X	X	X	X
benzene	X	X	X	X	X	X	X	X	X	X
1-(alkyl, acyc) benzene		X	X	X	X	X	X	X	X	X
1,3-dimethyl-benzene		X	X	X	X	X		X		
toluene		X	X	X	X	X		X		X
1-carbonyl-4-hydroxy-benzene	X									

Feature	Ethanone-BZT	sButBu-BZT	ditBu-BZT	ditPe-BZT	ditOc-BZT	MeEtPhMeBu-BZT	diMeEtPh-BZT	tBuPr Acid-BZT	Bisoctrizole	Oc-NTZ
methyl-ketone	X									
ketone	X									
1-benzyl benzene						X				
monosubstituted benzene						X				
1-hydroxy-4-(3-oxopropyl)-benzene								X		
alkyl, acyc-carboxylic acid								X		
carboxy								X		
alkyl, acyc-ketone	X									

The 1,4-benzene substitution pattern where one substituent was a hydroxyl moiety (i.e., 1-alkyl-4-hydroxy benzene, 1-carbonyl-4-hydroxy benzene, and 1-hydroxy-4-3(oxopropyl)benzene was identified as the structural feature that contributed the greatest to the predicted activity. The presence of a carbonyl group (e.g., ketone or alkyl, acyc-carboxylic acid features) also positively contributed to the predicted effects. The 1-(alkyl, acyc) benzene moiety had conflicting effects on the evaluated in chemicals. For some compounds, the presence of the moiety was identified as a positive feature (e.g., diMeEtPh-BZT) while for others it was identified as a negative feature (e.g., ditBu-BZT). In both cases, the predicted contribution to the overall effect was slight. [ILS Note: The lack of feature identification in some evaluated compounds is unclear. For example, the 1,3-dimethylbenzene moiety was identified in MeEtPhMeBu-BZT, but not in diMeEtPh-BZT. At least one substituent on the phenol ring was 1,1-dimethyl-ethylbenzene.]

The number of structurally similar chemicals for the positive compounds ranged from one to four; these are provided in the table below.

Structurally Similar Chemicals	Ethanone-BZT	sButBu-BZT	ditBu-BZT	ditPe-BZT	ditOc-BZT	MeEtPh MeBu-BZT	diMeEt Ph-BZT	tBuPrAcid-BZT	Bisoctrizole	Oc-NTZ
phenol		X	X	X	X	X				X
bisphenol A		X	X	X	X	X	X		X	X
LS-187694-copy-1*								X		
tyrosine								X		
oxaprozin								X		
2-(butan-2-yl)-4,6-dinitrophenol		X								
4-[4-(4-hydroxyphenyl)hexan-3-yl]phenol		X	X	X	X					X

Structurally Similar Chemicals	Ethanone-BZT	sButBu-BZT	ditBu-BZT	ditPe-BZT	ditOc-BZT	MeEtPh MeBu-BZT	diMeEt Ph-BZT	tBuPrAcid-BZT	Bisoctrizole	Oc-NTZ
benzene-1,4-diol			X	X	X					X
2-benzoyl-5-methoxy phenol	X									

*The structure of the structurally similar chemical is unclear, therefore the common and/or scientific name were not sought.

Carcinogenicity

This class of chemicals was evaluated in two sets of carcinogenicity endpoint models; seven are rodent models based on the two-year rodent bioassays and four are cell transformation *in vitro* assay models. The sensitivity and specificity of the rodent models range from 32.5% to 44.7% and 90.2% to 95.1%, respectively. The sensitivity and specificity of the *in vitro* models range from 87.8% to 93.9% and 22.5% to 55.8%, respectively.

All the compounds were either predicted to be negative or were identified as not in domain in all of the *in vivo* rodent models. There was a single *in vitro* model where ≥7 tested chemicals were predicted to be positive, C3H10T1-2 (22 predicted positive). The table below provides the predicted probabilities for the model. The percentage contribution of the features and physico-chemical properties evaluated are also provided.

	ditBu-BZT	ditBu-ClBZT	tBu-ClBZT	Allyl-BZT	Bumetrizole	DoM-BZT	ditPe-BZT	sButBu-BZT	diMeEtPh-BZT	ditOc-BZT	MeEtPhMeBu-BZT
Positive Prediction Value	0.752	0.746	0.776	0.756	0.754	0.694	0.72	0.728	0.745	0.702	0.711
% Feature contribution	2.174%	3.924%	7.955%	1.545%	1.814%	19.42%	8.909%	6.705%	34.08%	14.42%	36.38%
% Property contribution	97.83%	96.71%	92.04%	98.46%	98.19%	80.58%	91.09%	93.3%	65.92%	85.58%	63.62%

	tBuPrOcEst-ClBZT	tBuPrHexEst-BZT	tBuPrOcEst-BZT	tBuPrMeEst-BZT	tBuPrAcid-BZT	MeEtMeBu-CF_3BZT	Oc-NTZ	OcOx-BZT	Bisoctrizole	Octrizole	tBu-BZT
Positive Prediction Value	0.628	0.664	0.629	0.641	0.706	0.638	0.732	0.679	0.679	0.741	0.777
% Feature contribution	33.01%	29.88%	32.25%	9.241%	16.64%	28.83%	16.93%	33.61%	49.37%	-43.09%	7.81%
% Property contribution	66.99%	70.12%	67.75%	90.76%	83.36%	71.17%	83.07%	66.39%	50.63%	143.1%	92.19%

The table below list of the structural features identified as contributing to the activity of the noted chemical and the percentage.

Feature	ditBu-BZT	ditBu-ClBZT	tBu-ClBZT	Allyl-BZT	Bumetrizole	DoM-BZT	ditPe-BZT	sButBu-BZT	diMeEtPh-BZT	ditOc-BZT	MeEtPhMeBu-BZT
1-benzyl benzene									X		X
1,1-diaryl methane									X		X
1,1-diphenyl methane									X		X
propane	X	X	X	X	X	X	X	X	X	X	X
1,3-dialkyl benzene	X	X		X	X	X	X	X	X	X	X
propylbenzene						X	X	X		X	X
butane						X	X	X		X	X
2-methylpentane										X	X
octane						X					
alkyl, acyc-carbonyl											
butanoic acid											
alkyl carboxylate											
alkyl, acyc-carboxylate											
O-methyl oxycarbonyl											
1-methoxy hexane											
alkyl, acyc-carbonyl											
alkyl ether											
aryl ether											

Feature	ditBu-BZT	ditBu-ClBZT	tBu-ClBZT	Allyl-BZT	Bumetrizole	DoM-BZT	ditPe-BZT	sButBu-BZT	diMeEtPh-BZT	ditOc-BZT	MeEtPhMeBu-BZT
phenyl ether											
1-alkoxy benzene											
methoxy benzene											
alkyl, acyc-ether											
1-methoxy heptanes											
gem dihalide											
trifluoromethyl											

Feature	tBuPrOcEst-ClBZT	tBuPrHexEst-BZT	tBuPrOcEst-BZT	tBuPrMeEst-BZT	tBuPrAcid-BZT	MeEtMeBu-CF_3BZT	Oc-NTZ	OcOx-BZT	Bisoctrizole	Octrizole	tBu-BZT
1-benzyl benzene						X			X		
1,1-diaryl methane						X			X		
1,1-diphenyl methane						X			X		
propane	X	X	X	X	X	X	X	X	X	X	X
1,3-dialkyl benzene	X	X	X	X	X	X			X		
propylbenzene	X	X	X	X	X	X	X		X	X	
butane	X	X	X	X	X	X	X	X	X	X	
2-methylpentane						X	X		X	X	
octane	X		X					X			
alkyl, acyc-carbonyl				X	X						

Feature	tBuPrOcEst-ClBZT	tBuPrHexEst-BZT	tBuPrOcEst-BZT	tBuPrMeEst-BZT	tBuPrAcid-BZT	MeEtMeBu-CF_3BZT	Oc-NTZ	OcOx-BZT	Bisoctrizole	Octrizole	tBu-BZT
butanoic acid	X	X	X	X	X						
alkyl carboxylate	X	X	X	X							
alkyl, acyc-carboxylate	X	X	X	X							
O-methyl oxycarbonyl				X							
1-methoxy hexane	X	X	X					X			
alkyl, acyc-carbonyl	X	X	X								
alkyl ether								X			
aryl ether								X			
phenyl ether								X			
1-alkoxy benzene								X			
methoxy benzene								X			
alkyl, acyc-ether								X			
1-methoxy heptane	X		X					X			
gem dihalide						X					
trifluoromethyl						X					

As was shown in the above, the contribution of physico-chemical properties to the overall prediction value was greater than the structural features present in this class of compounds. The contribution of physico-chemical properties ranged from 50.63 to 143.1%. Of the 21 chemicals predicted to have activity, physico-chemical properties were identified as the greatest contributing factor to the predicted activity for 17 chemicals. In reviewing these chemicals, the presence of hydrogen bond acceptors was identified as the greatest positive contributing factor for 14 chemicals. For those compounds where structural elements were identified as being the largest contributor to the predicted positive activity, the structural motif of a di-aryl substituted methane was identified as being the largest contributors.

All the compounds, except OcOx-BZT, identified as single chemical as being structurally similar: 3,5-di-*tert*-butyl-4-hydroxytoluene. OcOx-BZT identified anthralin as being structurally similar.

Human Adverse Effects

Adverse cardiological, hepatobiliary, and urinary tract effects were evaluated in 24 models.

Adverse Cardiological

Thirteen models predicted cardiac endpoints, including: conduction disorders, coronary artery disorders, myocardial infarct disorders, palpitations, and rate rhythm disorders. The sensitivity and specificity of the models range from 32.1% to 65.7% and 85.8% to 93.6%, respectively. There was a single model where ≥7 tested chemicals were predicted to be positive, palpitations (7 predicted positive).

The table below provides the predicted probabilities for the overall model and the four sub-models. The percentage contribution of the features and physical-chemical properties evaluated, for the overall model, are also provided.

Positive Prediction Value	Bumetrizole	tBu-ClBZT	ditBu-ClBZT	tBuPrMeEst-BZT	tBuPrHexEst-BZT	tBuPrOcEst-BZT	tBuPrOcEst-ClBZT
Overall	0.52	0.5378	0.544	0.512	0.5955	0.6085	0.6875
Sub-model A	0.277	0.275	0.271	n.p.	n.p.	n.p.	n.p.
Sub-model B	0.634	0.631	0.636	n.p.	n.p.	n.p.	n.p.
Sub-model C	0.651	0.729	0.753	0.63	0.742	0.759	0.829
Sub-model D	0.518	0.516	0.516	0.394	0.449	0.458	0.546
% Feature contribution	104.3%	104.4%	103.0%	110.0%	118.5%	116.3%	103.3%
% Property contribution	-4.341%	-4.376%	-2.976%	-10.04%	-18.51%	-16.32%	-3.312%

Abbreviation: n.p. = not provided

The table below lists the structural features identified as contributing to the activity of the noted chemical and the percentage. [ILS Note: Since the endpoint is composed four sub-models, the structural features identified in the overall model are provided below.]

Feature	tBu-ClBZT	Bumetrizole*	ditBu-ClBZT	tBuPrMeEst-BZT	tBuPrHexEst-BZT	tBuPrOcEst-BZT	tBuPrOcEst-ClBZT
t-butylbenzene	X	X	X	X	X	X	X
chlorobenzene	X	X	X				X
1-(alkyl, acyc)-benzene	X	X	X	X	X	X	X
phenylhalide	X	X	X				X
propane	X	X	X				
toluene	X	X	X	X	X	X	X
oxybenzene	X	X	X	X	X	X	X
hydroxybenzene	X	X	X	X	X	X	X
alkyl, acyc-carbonyl				X	X	X	X
O-methyl-oxycarbonyl				X			

*For this chemical, a toluene moiety was identified twice as a contributing structural element. In one entry, the moiety was positively associated with activity while another entry indicates that it was negatively associated with activity. The different sub-models also showed differences in the contribution of toluene to the evaluated activity. For sub-models A and D, toluene was positive associated with activity. Toluene was negatively associated with activity in sub-model B. In sub-model C, the moiety was positively and negatively associated with activity.

For all the chemicals, the presence of the t-butylbenzene moiety was identified was the largest contributor to the proposed activity. For those chemicals with chlorine on the benzotriazole ring, that moiety was identified as being the second largest contributor to activity. However, its contribution was much smaller than compared to the t-butylbenzene moiety. The (alkyl, acyc)-benzene moiety was identified as being a large contributor to activity for those compounds without a chlorine substituent. The hydroxy substituent on the appended phenyl ring was identified as a structural feature present in all chemicals that was negatively associated with the evaluated activity.

The number of structurally similar chemicals for the positive compounds ranged from two to thirteen; these are provided in the table below.

Structurally Similar Chemicals	tBu-ClBZT	Bumetrizole	ditBu-ClBZT	tBuPrMeEst-BZT	tBuPrHexEst-BZT	tBuPrOcEst-BZT	tBuPrOcEst-ClBZT
4-chlorophenol	X	X	X				X
3,5-di-tert-butyl-4-hydroxytoluene	X	X	X	X	X	X	
2,2'-methylenebis(4-chlorophenol)	X	X	X				X
pentachlorophenol	X	X	X				
probucol		X	X				
chloroxine	X		X				

Structurally Similar Chemicals	tBu-ClBZT	Bumetrizole	ditBu-ClBZT	tBuPrMeEst-BZT	tBuPrHexEst-BZT	tBuPrOcEst-BZT	tBuPrOcEst-ClBZT
5-chlorobenzoxazolinone	X		X				
4-hexyl-m-xylene	X		X				
triclosan	X						
phenol	X						
thymol	X						
chlorquinaldol	X						
3-t-butyl-4-hydroxyanisole	X						
clioquinol	X						
estradiol cypionate				X	X	X	
estradiol enanthate				X	X	X	
estradiol valerate				X	X	X	

Adverse Heptatobiliary
Five models predicted hepatobiliary endpoints, including: bile duct, gall bladder, liver jaundice, liver acute damage, and liver enzyme release. The sensitivity and specificity of the models range from 23.9% to 51.7% and 91.4% to 97.9%, respectively. None of the chemicals evaluated were identified as positive in any of the models evaluated.

Adverse Urinary
Six models predicted urinary endpoints, including: bladder, blood in urine, kidney, kidney function tests, nephropathy, and urolithiasis. The sensitivity and specificity of the models range from 34.5% to 55.8% and 89.2% to 96.5%, respectively. None of the chemicals evaluated were identified as positive in any of the models evaluated.

11.0 Online Databases and Secondary References Searched

11.1 Online Databases

National Library of Medicine Databases
PubMed
ChemIDplus – chemical information database that provides links to other databases such as CCRIS, DART, GENE-TOX, HSDB, IRIS, and TRI. A full list of databases and resources searched are available at http://www.nlm.nih.gov/databases/.

STN International Files

AGRICOLA	FROSTI
BIOSIS	FSTA
BIOTECHNO	IPA
CABA	MEDLINE

EMBASE	Registry
ESBIOBASE	TOXCENTER

Information on the content, sources, file data, and producer of each of the searched STN International Files is available at http://www.cas.org/support/stngen/dbss/index.html.

Government Printing Office
Code of Federal Regulations (CFR)

11.2 Secondary References

None used

12.0 References

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- Drometizole: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=17113&loc=ec_rcs
- tBu-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=76605&loc=ec_rcs
- tBu-ClBZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=3014188&loc=ec_rcs
- Octrizole: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=62485&loc=ec_rcs
- EtOH-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=688251&loc=ec_rcs
- Ethanone-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=158568&loc=ec_rcs
- DoM-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=86375&loc=ec_rcs
- sButBu-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=118327&loc=ec_rcs
- Bumetrizole: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=62531&loc=ec_rcs
- ditBu-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=77455&loc=ec_rcs
- ditBu-ClBZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=77470&loc=ec_rcs
- ditPe-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=33263&loc=ec_rcs
- ditOc-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=116809&loc=ec_rcs
- MeEtPhMeBu-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=9803353&loc=ec_rcs
- diMeEtPh-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=112412&loc=ec_rcs
- tBuPrAcid-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=158619&loc=ec_rcs
- tBuPrMeEst-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=93481&loc=ec_rcs
- tBuPrHexEst-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=3086183&loc=ec_rcs
- tBuPrOcEst-ClBZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=174297&loc=ec_rcs
- tBu(C_{7-9})Est-BZT: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=86220&loc=ec_rcs
- Bisoctrizole: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=3571576&loc=ec_rcs
- Oc-NTZ: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=119736&loc=ec_rcs

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- 2-(2H-Benzotriazol-2-yl)-4-(1,1-dimethylethyl)phenol; RN 3147-76-0
- 2-(5-Chloro-2H-benzotriazol-2-yl)-4-(1,1-dimethylethyl)phenol; RN 3287-17-0
- Octrizole; RN 3147-75-9
- 3-(2H-Benzotriazol-2-yl)-4-hydroxybenzeneethanol; RN 96549-95-0
- 1-[3-(2H-Benzotriazol-2-yl)-4-hydroxyphenyl]ethanone; RN 83741-30-4
- 2-(2H-Benzotriazol-2-yl)-4-(1,1-dimethylethyl)-6-(1-methylpropyl)phenol; RN 36437-37-3
- Bumetrizole; RN 3896-11-5
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- 2-(5-Chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)phenol; RN 3864-99-1
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- 2-(2H-Benzotriazol-2-yl)-4,6-bis(1,1,3,3-tetramethylbutyl)phenol; RN 70693-49-1
- 2-(2H-Benzotriazol-2-yl)-6-(1-methyl-1-phenylethyl)-4-(1,1,3,3-tetramethylbutyl)phenol; RN 73936-91-1
- 2-(2H-Benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol; RN 70321-86-7
- 3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid; RN 84268-36-0
- 3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, methyl ester; RN 84268-33-7
- 3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, 1,6-hexanediyl ester; RN 84268-08-6
- 3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-benzenepropanoic acid, C_{7-9}-branched and linear alkyl esters; RN 127519-17-9
- Bisoctrizole; RN 103597-45-1
- 2-(2H-Naphtho(1,2-*d*)triazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol; RN 27876-55-7

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- 2-(2H-Benzotriazol-2-yl)phenol; RN 10096-91-0
- 4-(2-Methacryloyloxyethyl)-2-(2H-benzotriazol-2-yl)phenol; RN 96478-09-0 [Entered STN on May 25, 1985]
- 2-(2H-Benzotraizol-2-yl)-4-methyl-6-(2-propenyl)phenol; RN 2170-39-0
- 2-(2H-Benzotriazol-2-yl)-6-dodecyl-4-methylphenol; RN 23328-53-2
- 2-(1-Methyl-1-phenylethyl)-4-(1,1,3,3-tetramethylbutyl)-6-[5-(trifluoromethyl)-2H-benzotriazol-2-yl]phenol; RN 207738-63-4 [Entered STN on June 28, 1998]
- 3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, octyl ester; RN 84268-23-5
- 3-(5-Chloro-2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, octyl ester; RN 83044-89-7
- 2-(2H-Benzotriazol-2-yl)-5-(octyloxy)phenol; RN 3147-77-1
- Polyethylene glycol mono-3-(3-(2H-benzotriazol-2-yl)-5-*tert*-butyl-4-hydroxyphenyl)-1-oxopropyl ether; RN 104810-48-2 [Entered STN on October 25, 1986]
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Appendix A: Units and Abbreviations

ºC = degrees Celsius
µg/g = microgram(s) per gram
µg/kg = microgram(s) per kilogram
µg/mL = microgram(s) per milliliter
µM = micromolar
µmol/min= micromole(s) per minute
CASRN = Chemical Abstracts Service Registry Number
CF = caffeine
CFR = Code of Federal Regulations
CHO = Chinese hamster ovary
CID = chemical identification
EPA = U.S. Environmental Protection Agency
EtOH = ethanol
F = female(s)
FDA = U.S. Food and Drug Administration
G = gram(s)
g/cm^3 = gram(s) per cubic centimeter
g/kg = gram(s) per kilogram
GC-MS = gas chromatography-mass spectrometry
GC-MS/MS = gas chromatography with tandem mass spectrometry
GD = gestation day(s)
HPLC = high performance liquid chromatography
ILS = Integrated Laboratory Systems, Inc.
IC_{50} = half maximal inhibitory concentration
IsoPrOH = isopropanol
IUR = Inventory Update Reporting
LC_{50} = lethal concentration for 50% of test animals
LD_{50} = lethal dose for 50% of test animals
M = male(s)
MeOH = methanol
mg = milligram(s)
mg/kg = milligram(s) per kilogram
mg/L = milligram(s) per liter
mg/m^3 = milligram(s) per cubic meter
mol. wt. = molecular weight
mp = methanolic eluates from polymerized specimens
MSW RDF = municipal solid waste refuse-derived fuel
mu = methanolic eluates from unpolymerized specimens
N/A = not available
ND = not detected
n.p. = not provided
ng/g = nanogram(s) per gram
ng/L = nanogram(s) per liter
ng/mL = nanogram(s) per milliliter
NIOSH = National Institute for Occupational Safety and Health

NOAEL = no observed adverse effect level
NOEL = no observed effect level
NTP = National Toxicology Program
PET = polyethyleneterephthalate
pg = picogram(s)
PMID = PubMed identification
ppb = part(s) per billion
ppm = part(s) per million
ppt = part(s) per trillion
S9 = metabolic activation
SNUR = Significant New Use Rule
STP = sewage treatment plant
TD_{Lo} = lowest toxic dose
UDP = uridine-5'-diphosphosphate
UV = ultraviolet
wt.% = weight percent

Appendix B: Description of Search Strategy and Results

Octrizole

Preliminary searches on octrizole were conducted at www.inchem.org and in National Library of Medicine files ChemIDplus (http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp), HSDB (http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB), and PubMed (http://www.ncbi.nlm.nih.gov/pubmed/) on August 17 and 19, 2010. STN International files MEDLINE, AGRICOLA, CABA, IPA, BIOSIS, TOXCENTER, FSTA, FROSTI, EMBASE, ESBIOBASE, and BIOTECHNO were searched simultaneously on August 18, 2010. The keywords and strategy are shown below. RTECS and the REGISTRY files were searched on August 17, 2010 based on the CAS Registry Numbers.

```
                SET DUPORDER FILE
L1            28 S 3147-75-9
L2            25 S OCTRIZOLE OR OCTRIZOL OR OCTRIZOLUM OR ((CYASORB OR
                   CHISORB OR UV OR (SPECTRA (W) SORB)) (2W) 5411) OR
                   (SEESORB (W) 709) OR (SUMISORB (W) 340) OR ((TINUVIN
                   OR UV) (W) 329) OR (VIOSORB (W) 583) OR (UVINUL (W)
                   3029)OR (KEMISORB (W) 79) OR (EVERSORB (W) 72) OR (JF
                   (W) 83)
L3             3 S HYDROXY (3W) (T OR TERT) (2W) OCTYLPHENYL (5W)
                   (BENZOTRIAZOLE OR BENZTRIAZOLE)
L4             0 S (T OR TERT) (2W) OCTYL (3W) HYDROXYPHENYL (2W)
                   (BENZOTRIAZOLE OR BENZTRIAZOLE)
L5             9 S (BENZOTRIAZOL (10W) TETRAMETHYLBUTYL) (5A) PHENOL
L6             1 S (HYDROXY (8W) TETRAMETHYLBUTYL) (2W) PHENYL (2W)
                   BENZOTRIAZOLE
L7             0 S BENZOTRIAZOLYL (3W) (TERT OR T) (2W) OCTYLPHENOL
L8            51 S (L1 OR L2 OR L3 OR L4 OR L5 OR L6 OR L7)
L9            42 DUP REMOVE L8 (9 DUPLICATES REMOVED)
                ANSWERS '1-2' FROM FILE MEDLINE
                ANSWERS '3-4' FROM FILE BIOSIS
                ANSWERS '5-37' FROM FILE TOXCENTER
                ANSWER '38' FROM FILE FSTA
                ANSWERS '39-42' FROM FILE EMBASE
L10           42 SORT L9 1-42 TI
               SAVE L10 X074OOct/A
```

Sixteen full records were downloaded from the 42 records on octrizole (12 from TOXCENTER, 2 from BIOSIS, and 1 each from EMBASE and MEDLINE).

Octrizole Analogs

Ten analogs (see Section 10.0 of report for names and structures) were searched in conjunction with octrizole. RTECS and Registry files were searched on August 17 and 19, 2010. Preliminary searches were conducted on each of the octrizole analogs at www.inchem.org and in National Library of Medicine files ChemIDplus (http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp), HSDB (http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB), and PubMed (http://www.ncbi.nlm.nih.gov/pubmed/). STN International files MEDLINE, AGRICOLA, CABA, IPA, BIOSIS, TOXCENTER, FSTA, FROSTI, EMBASE, ESBIOBASE, and BIOTECHNO were searched simultaneously on August 18, 19, and 25, 2010. Searches conducted are provided below and the number of records retrieved are provided in the table following the reproduced searches.

August 18, 2010

```
                SET DUPORDER FILE
L1          237 S 2440-22-4
L2          693 S DROMETRIZOLE OR (BENAZOL (W) (II OR P)) OR (BT (W) 1)
                  OR (JF (W) (77#)) OR (KEMISORB OR EVERSORB (W) 71) OR
                  (LA (W) 32) OR (LOWLITE (W) 55) OR (SEESORB (W) 701)
L3          343 S (SUMISORB (W) 200) OR ((TINUVIN OR TIN OR POREX OR
                  BENAZOL) (W) P) OR (UV (W) ((ABSORBER (W) 1) OR P))
                  OR (UVA (W) P) OR (UVASORB (W) SV) OR (UVINUL (W)
                  3033P) OR (VIOSORB (W) 520) OR (DAINSORB (W) T (W) 1)
L4            9 S BENZOTRIAZOL (5W) (METHYLPHENOL OR (METHYL (2W)
                  PHENOL) OR CRESOL)
L5            3 S (BENZOTRIAZOL (5W) METHYL) (8A) PHENOL
L6           28 S (BENZOTRIAZOL) (8A) PHENOL
L7            0 S HYDROXY (5W) (METHYL OR METHYLPHENYL OR (METHYL
                  (2W) PHENYL)) (5W) BENZOTRIAZOL#
L8           96 S HYDROXY (5W) (METHYL OR METHYLPHENYL OR (METHYL (2W)
                  PHENYL))
L9            0 S (METHYL (4W) HYDROXYPHEYL) (2W) BENZOTRIAZOLE
L10           3 S (METHYL (4W) HYDROXYPHENYL) (2W) BENZOTRIAZOLE
L11           0 S L1-L6 AND L8 AND L10
L12        1129 S L1-L6 OR L8 OR L10
L13         666 DUP REM L12 (463 DUPLICATES REMOVED)
L14         666 SORT L13 1-666 TI
                SAVE L14 X0740DROM/A
```

August 19, 2010

```
                SET DUPORDER FILE
L1           84 S 103597-45-1
L2          109 S BISOCTRIZOLE OR BISOCTYLTRIAZOLE OR (EVERSORB (W) 78)
                  OR (((ADEKASTAB OR ADK OR MARK) (2W) LA) (W) 31) OR
                  (MIXXIM (W) BB (W) 100) OR (TINOSORB (W) M) OR
                  (TINUVIN (W) 360) OR (LA (W) 31) OR (JF (W) 832)
L3            1 S METHYLENEBIS (8W) TETRAMETHYLBUTYL (5W)
                  (BENZOTRAIZOLYLPHENOL OR BENZOTRIAZOL)
L4            2 S METHYLENEBIS (5W) (BENZOTRIAZOLYL OR BENZOTRIAZOL OR
                  BENZOTRIAZOLE) (10W) TETRAMETHYLBUTYL
L5            0 S METHYLENEBIS (3W) HYDROXYL (3W) BENZOTRIAZOL (4W)
                 (TERT OR T) (2W) (OCTYLPHENYL OR OCTYL (W) PHENYL)
L6            0 S METHYLENEBIS (3W) HYDROXYL (3W) BENZOTRIAZOL (4W)
                  (TERT OR T) (2W) (OCTYLPHENYL OR (OCTYL (W) PHENYL))
L7            0 S BIS (3W) HYDROXY (3W) (TERT OR T) (2W) OCTYL (3W)
                  BENZOTRIAZOL (5W) METHANE
L8            0 S METHYLENEBIS (3W) HYDROXY (3W) BENZOTRIAZOL (4W)
                  (TERT OR T) (2W) (OCTYLPHENYL OR (OCTYL (W) PHENYL))
L9          168 S L1-L3
L10         131 DUP REMOVE L9 (37 DUPLICATES REMOVED)
L11         131 SORT L10 1-131 TI
                SAVE L11 X0740BISOCT/A

                SET DUPORDER FILE
L1           45 S 3846-71-7
L2            4 S (EVERSORB (W) 77) OR (KEMISORB (W) 75) OR (SEESORB
                        (W) 705) OR (SUMISORB (W) 320) OR (TINUVIN (W) 320)
                        OR (VIOSORB (W) 582)
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L3             50 S HYDROXY (6W) (TERT OR T) (W) (BUTYLPHENYL OR BUTYL
                    (W) PHENYL) (5W) BENZOTRIAZOLE
L4             12 S (((TERT OR T) (W) BUTYL) (2W) HYDROXYPHENYL) (5W)
                    BENZOTRIAZOLE
L5              0 S ((BENZOTRIAZOL OR BENZOTRIAZOLYL) (10W) (TERT OR T))
                    (W) (BUTYLPHENOL OR (BUTYL (W) PHENOL))
L6              1 S PHENOL (5A) (BENZOTRIAZOL (10W) (DIMETHYLETHYL OR
                    ((TERT OR T) (W) BUTYL)))
L7             85 S L1-L6
L8             42 DUP REMOVE L7 (43 DUPLICATES REMOVED)
L9             50 S 25973-55-1
L10            30 S ((CHISORB OR UV OR TIN OR TINUVIN) (W) 328) OR
                    (CYASORB (2W) 2337) OR ((EVERSORB OR UV OR KEMISORB)
                    (W) 74) OR (LOWILITE (W) 28) OR (SEESORB (W) 704) OR
                    (SUMISORB (W) 350) OR (VIOSORB (W) 591)
L11             6 S (((HYDROXY (5W) (TERT OR T)) (W) (AMYLPHENYL OR
                    PENTYLPHENYL) (4W) BENZOTRIAZOLE
L12             2 S (((DI (2W) (TERT OR T)) (3W) (AMYL OR PENTYL)) (2W)
                    HYDROXYPHENYL) (4W) BENZOTRIAZOLE
L13             3 S ((BENZOTRIAZOL (7W) DI) (W) (TERT OR T)) (W)
                    (PENTYLPHENOL OR PENTYL)
L14             1 S (BENZOTRIAZOL (10W) DIMETHYLPROPYL) (5A) PHENOL
L15            68 S L9-L13
L16            55 DUP REMOVE L15 (13 DUPLICATES REMOVED)
L17             0 S 73936-91-1
L18             0 S (CHISORB (W) 5228) OR (TINUVIN (W) 928)
L19             0 S (DIMETHYLBENZYL OR PHENYLETHYL) (10W)
                    ((TETRAMETHYLBUTYL (2W) PHENYL (4W) BENZOTRIAZOLE) OR
                    (TETRAMETHYLBUTYL (4W) BENZOTRIAZOL (4W) PHENOL))
L20             3 S HYDROXY (8W) ((OCTYLPHENYL (4W) BENZOTRIAZOLE) OR
                    (DIMETHYLBENZYL (4W) (TERT OR T) (W) OCTYLPHENYL (4W)
                    BENZOTRIAZOLE))
L21             0 S "PHENOL, 2-(2H-BENZOTRIAZOL-2-YL)-6-(1-METHYL-1-
                    PHENYLETHYL)-4- (1,1,3,3-TETRAMETHYLBUTYL)-"
L22             0 S PHENOL (4A) (((BENZOTRIAZOL (8W) METHYL) (2W)
                    PHENYLETHYL) (8W) TETRAMETHYLBUTYL)
L23             3 S L17-L21
L24             3 DUP REMOVE L23 (0 DUPLICATES REMOVED)
L25             3 SORT L24 1-3 TI
                  SAVE L25 X0740TIN928/A
L26            42 SORT L8 1-42 TI
                  SAVE L26 X0740TIN320/A
L27            55 SORT L16 1-55 TI
                  SAVE L27 X0740TIN328/A
L28            20 S 70321-86-7
L29            99 S (BENZOTRIAZOLE (W) BT) OR ((EVERSORB OR LOWILITE OR T
                    OR TINUVIN OR UV) (W) 234#) OR (EVERSORB (W) 76) OR
                    (TINUVIN (W) 900) OR (UVINUL (W) 3034)
L30             9 S (BENZOTRIAZOL (8W) BIS) (5W) ((DIMETHYLBENZYL (W)
                    PHENOL) OR (1 (W) METHYL (W) 1 (W) PHENYLETHYL))
L31             3 S ((((HYDROXY (3W) BIS) (5W) DIMETHYLBENZYL) (2W)
                    PHENYL) (4W) BENZOTRIAZOLE)
L32             0 S (DIMETHYLBENZYL (2W) HYDROXYPHENYL) (W) BENZOTRIAZOLE
L33             0 S ((HYDROXY (8W) (CUMYLPHENYL OR (CUMYL (W) PHENYL)))
                    (4W) BENZOTRIAZOLE)
L34             0 S (((((1 (W) METHYL) (W) 1) (W) PHENYLETHYL) (2W)
                    HYDROXYPHENYL) (W) BENZOTRIAZOLE)
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L35          112 S L28-L34
L36           46 DUP REMOVE L35 (66 DUPLICATES REMOVED)
L37           46 SORT L36 1-46 TI
                 SAVE L37 X0740TIN900/A
L38            6 S 84268-33-7
L39           24 S TINUVIN (W) 1130
L40            1 S (BENZENEPROPANOIC (W) ACID) (4A) ((((BENZOTRIAZOL
                   (8W) 1) (W) 1) (W) DIMETHYLETHYL) (3W) HYDROXY)
L41            0 S (((((TERT OR T) (W) BUTYL) (W) HYDROXY) (10W)
                   METHOXYCARBONYLETHYL) (4W) BENZOTRIAZOLE)
L42            2 S (((BENZOTRIAZOL (8W) 4) (W) HYDROXYPHENYL) (2W)
                   PROPIONATE)
L43           31 S L38-L42
L44           28 DUP REMOVE L43 (3 DUPLICATES REMOVED)
L45           28 SORT L44 1-28 TI
                 SAVE L45 X0740TRIAEST/A

                 SET DUPORDER FILE
L1            58 S 3864-99-1
L2           258 S ((HISORP OR HISORB OR TINUVIN OR TNV OR UV) (W) 327)
                   OR (CYASORB (2W) 5357) OR (EVERSORB (W) 75) OR
                   (KEMISORB (W) 72) OR (LA (W) 34) OR (LOWILITE (W) 27)
                   OR (SEESORB (W) 702) OR (UV (W) 2) OR (UV (3W) 607)
                   OR (VIOSORB (W) 580)
L3            57 S ((HISORP OR HISORB OR TINUVIN OR TNV OR UV) (W) 327)
                   OR (CYASORB (2W) 5357) OR (EVERSORB (W) 75) OR
                   (KEMISORB (W) 72) OR (LA (W) 34) OR (LOWILITE (W) 27)
                   OR (SEESORB (W) 702) OR (UV (3W) 607) OR (VIOSORB (W)
                   580)
L4            55 S ((HYDROXY (10W) (TERT OR T)) (W) BUTYLPHENYL) (4W)
                   (CHLOROBENZOTRIAZOLE OR (CHLORO (4W) BENZOTRIAZOLE)
                   OR BENZOTRIAZOLE)
L5            41 S (((DI (W) (TERT OR T)) (W) BUTYL) (3W) HYDROXYPHENYL)
                   (4W) (CHLOROBENZOTRIAZOLE OR (CHLORO (4W)
                   BENZOTRIAZOLE) OR BENZOTRIAZOLE)
L6            10 S ((DI (W) (TERT OR T)) (W) BUTYL) (5W)
                   (CHLOROBENZOTRIAZOL OR (CHLORO (4W) BENZOTRIAZOL))
L7             0 S ((CHLORO (4W) BENZOTRIAZOL) (10W) DIMETHYLETHYL) (5A)
                    PHENOL
L8           173 S L1 OR L3 OR L4 OR L5 OR L6
L9            88 DUP REMOVE L8 (85 DUPLICATES REMOVED)
L10           88 SORT L9 1-88 TI
                 SAVE L10 X0740TIN327/A
L11          861 S 3896-11-5
L12          853 S ((ADK OR LA OR MARK LA) (4W) 36##) OR ((TIN OR
                   TINUVIN OR TNV OR UV) (W) 326) OR ((VIOSORB OR VS)
                   (W) 550) OR BUMETRIZOLE OR (EVERSORB (W) 73) OR
                   (LOWILITE (W) 26)
L13          838 S ((ADK OR LA OR MARK LA) (4W) 36##) OR ((TIN OR
                   TINUVIN OR TNV) (W) 326) OR ((VIOSORB OR VS) (W) 550)
                   OR BUMETRIZOLE OR (EVERSORB (W) 73) OR (LOWILITE (W)
                   26)
L14           18 S (KEMISORB (W) 73) OR (SEESORB (W) 703) OR (SUMISORB
                   (W) 300) OR (TINOGARD (W) AS) OR (TOMISORB (W) 600)
                   OR (J (W) 395) OR (JC (W) 30S) OR (JF (W) 79) OR
                   (BENAZOL (W) PBKH) OR (CIBATEX (W) LF)
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L15          33 S (((HYDROXY (3W) (TERT OR T)) (W) BUTYL) (3W)
                  METHYLPHENYL) (4W) (CHLOROBENZOTRIAZOLE OR (CHLORO
                  (4W) BENZOTRIAZOLE) OR BENZOTRIAZOLE)
L16           1 S (((TERT OR T) (W) BUTYL) (4W) ((HYDROXY (4W)
                  METHYLPHENYL) OR (METHYL (4W) HYDROXYPHENYL))) (4W)
                  (CHLOROBETNZOTRIAZOLE OR (CHLORO (4W) BENZOTRIAZOLE))
L17           0 S ((CHLORO (4W) BENZOTRIAZOL) (10W) DIMETHYLETHYL) (5A)
                  (PHENOL OR METHYLPHENOL)
L18           1 S ((((TERT OR T) (W) BUTYL) (5W) CHLORO) (4W)
                  BENZOTRIAZOL##) (5W) METHYLPHENOL
L19           0 S CRESOL (4A) ((((TERT OR T) (W) BUTYL) (5W) CHLORO)
                  (4W) BENZOTRIAZOL##)
L20           0 S (((CHLORO (4W) BENZOTRIAZOL) (5W) METHYL) (4W) ((TERT
                  OR T) (W) BUTYL)) (W) PHENOL
L21           0 S ((((CHLORO (4W) (TERT OR T)) (W) BUTYL) (3W) HYDROXY)
                  (3W) METHYLPHENYL) (2W) BENZOTRIAZOLE
L24        1700 S L11 OR L12 OR L14 OR L15 OR L16 OR L18
L25        1247 DUP REMOVE L24 (453 DUPLICATES REMOVED)
L26        1247 SORT L25 1-1247 TI
                SAVE L26 X0740BUMET/A
L27           0 S 70693-49-1
L28           6 S PHENOL (4A) (BENZOTRIAZOL (8W) (1 (W) 1 (W) 3 (W) 3
                (W) TETRAMETHYLBUTYL))
L29           6 DUP REMOVE L28 (0 DUPLICATES REMOVED)
L30           6 SORT L29 1-6 TI
                SAVE L30 X0740BTOCT/A
L31        1246 S 95-14-7
L32        1507 S ((1 (W) 2 (W) 3) (3W) (BENZOTRIAZOLE OR (TRIAZA (3W)
                  INDENE) OR TRIAZAINDENE)) OR (1H (2W) BENZOTRIAZOLE)
                  OR ((1 (W) 2) (2W) AMINOAZOPHENYLENE) OR ((2 (W) 3)
                  (2W) (DIAZAINDOLE OR AZIMIDOBENZENE OR AZIMINOBENZENE
                  OR (BENZENE (W) AZIMIDE))) OR BENZISOTRIAZOLE
L33          65 S (KEMITEC (W) TT) OR (M (W) 318) OR (RUSMIN (W) R) OR
                  (SEETEC (W) (BT OR (BT (W) R))) OR (VERZONE (W)
                  CRYSTAL)
L34          34 S (BLS (W) 1326) OR (BT (W) 120) OR ((C.V.I. OR CVI)
                  (W) LIQUID) OR (COBRATEC (W) ((35G OR 99) OR (D (W)
                  32 (W) 108))) OR ENTEK OR (IRGASTAB (W) I (W) 489) OR
                  (ISK (W) 3)
L35        2009 S L31-L34
L36        1652 DUP REMOVE L35 (357 DUPLICATES REMOVED)
L37        1652 SORT L36 1-1652 TI
                SAVE L37 X0740BZT/A
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                ACTIVATE X0740BUMET/A
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L1 (       861)SEA 3896-11-5
L2 (       853)SEA ((ADK OR LA OR MARK LA) (4W) 36##) OR ((TIN OR
                   TINUVIN OR T
L3 (        18)SEA (KEMISORB (W) 73) OR (SEESORB (W) 703) OR (SUMISORB
                   (W) 300
L4 (        33)SEA (((HYDROXY (3W) (TERT OR T)) (W) BUTYL) (3W)
                   METHYLPHENYL)
L5 (         1)SEA (((TERT OR T) (W) BUTYL) (4W) ((HYDROXY (4W)
                   METHYLPHENYL)
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L6 (          1)SEA ((((TERT OR T) (W) BUTYL) (5W) CHLORO) (4W)
                    BENZOTRIAZOL##)
L7 (       1700)SEA L1 OR L2 OR L3 OR L4 OR L5 OR L6
L8 (       1247)DUP REMOVE L7 (453 DUPLICATES REMOVED)
L9          1247 SOR L8 1-1247 TI
                ---------
L10           260 S ((ADK OR MARK LA) (3W) 36##) OR (LA (W) 36) OR ((TIN
                   OR TINUVIN OR TNV OR UV) (W) 326) OR ((VIOSORB OR VS)
                   (W) 550) OR BUMETRIZOLE OR (EVERSORB (W) 73) OR
                   (LOWILITE (W) 26)
L11         1081 S L1 OR L10
L12         1107 S L1 OR L3 OR L4 OR L5 OR L6 OR L10
                 SET DUPORDER FILE
L13          950 DUP REM L12 (157 DUPLICATES REMOVED)
L15          950 SORT L13 1-950 TI
                 DELETE X0740Bumet/A
                 SAVE L15 X0740Bumet/A
```

Full abstracts downloaded for each of the searched analogs

Chemical	Total Abstracts Downloaded	MEDLINE	BIOSIS	TOXCENTER	EMBASE	Additional Databases
95-14-7	41		6	33	2	
2440-22-4	38	5	4	17	11	1 FSTA
3846-71-7	11	6		5		
25973-55-1	5		1	4		
73936-91-1	0					
70321-86-7	3	1		1	1	
84268-33-7	7			7		
3864-99-1	7	3	1	3		
3896-11-5	16	9		4	1	1 AGRICOLA 1 FROSTI
70693-49-1	0					
103597-45-1	8	5	1	1		1 IPA

To minimize duplicate retrievals, initially selected titles were compared to previously retrieved abstracts to identify identical articles. Articles that were identified as referring to more than one of the evaluated chemicals were identified as such in EndNote and the selected article was not retrieved.

Selected Phenolic Benzotriazoles (more commonly known as Hydroxyphenylbenzotriazoles)
Simultaneous searches were done in STN International files MEDLINE, AGRICOLA, CABA, IPA, BIOSIS, TOXCENTER, FSTA, FROSTI, and EMBASE on different groups of compounds.

ESBIOSBASE and BIOTECHNO, which had been used in the 2010 search on Set 1, were included for only Set 1. Their online costs are much higher than those of most of the other databases and the additional cost, when query building was slower than usual, was not proportional to the gains. Unique records from ESBIOBASE and BIOTECHNO have seldom been retrieved on previous searches. Name fragments were from the lists of synonyms and trade names for each compound in its Registry record.

Set 1

Set 1 contained benzotriazoles that had been reviewed in the ILS 2010 Octrizole draft. Set 1 was searched on August 25,30, and 31, 2011. The search strategy used in 2010 (August 18) was repeated and results were limited to publication in 2010 and 2011. The online session history is duplicated below.

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L1          36 S 3147-75-9
L2          38 S OCTRIZOLE OR OCTRIZOL OR OCTRIZOLUM OR ((CYASORB OR CHISORB OR UV OR
                 (SPECTRA(W)SORB))(2W)5411) OR (SEESORB(W)709) OR (SUMISORB(W)340) OR
                 ((TINUVIN OR UV)(W)329) OR (VIOSORB(W)583) OR (UVINUL(W)3029) OR
                 (KEMSORB(W)79) OR (EVERSORB(W)72) OR (JF(W)83)
L3           0 S HYDROXY(3W)(T OR TERT)(2W)OCTYLPHENOL(5W)(BENZOTRIAZOLE OR
                 BENZTRIAZOLE)
L4           0 S (T OR TERT)(2W)OCTYL(3W)HYDROXYPHENYL(2W)(BENZOTRIAZOLE OR
                 BENZTRIAZOLE)
L5          12 S (BENZOTRIAZOL(10W)TETRAMETHYLBUTYL)(5A)PHENOL
L6           1 S (HYDROXY(8W)TETRAMETHYLBUTYL)(2W)PHENYL(2W)BENZOTRIAZOLE
L7          68 S L1-L6
               SET DUPORDER FILE
L8          53 DUP REM L7 (15 DUPLICATES REMOVED)
L9          16 S L8 AND (2010-2011)/PY
L10         16 SORT L9 1-16 TI
               SAVE L10 X0740OCT/A

L11        341 S 2440-22-4 OR DROMETRIZOLE
L12        587 S BENZOL(W)(II OR P) OR BT(W)1 OR JF(W)77# OR (KEMISORB OR EVERSORB)
                (W)71 OR LA(W)32 OR LOWLITE(W)55 OR SEESORB(W)701
L13         30 S BENAZOL(W)(II OR P)
L14        377 S SUMISORB(W)200 OR (TINUVIN OR TIN OR POREX OR BENAZOL)(W)P OR
                 UV(W)(ABSORBER(W)1 OR P) OR UVA(W)P OR UVASORB(W)SV OR UVINUL(W)3033P
                 OR VIOSORB(W)520 OR DAINSORB(W)T(W)1
L15         16 S BENZOTRIAZOL(5W)(METHYLPHENOL OR METHYL(2W)PHENYL OR CRESOL)
L16          5 S (BENZOTRIAZOL(5W)METHYL)(8A)PHENOL
L17         37 S BENZOTRIAZOL(8A)PHENOL
L18        103 S HYDROXY(5W)(METHYL OR METHYLPHENYL OR METHYL(2W)PHENYL)
                 (5W)BENZOTRIAZOL#
L19          3 S (METHYL(4W)HYDROXYPHENYL)(2W)BENZOTRIAZOLE
L20       1289 S L11-L19
L21        762 DUP REM L20 (527 DUPLICATES REMOVED)
L22         80 S L21 AND (2010-2011)/PY
L23         80 SORT L22 1-80 TI
               SAVE L23 X0740DROM/A

L24        107 S 103597-45-1 OR BISOCTRIZOLE OR BISOCTYLTRIAZOLE
L25        108 S EVERSORB(W)78 OR (ADEKASTAB OR ADK OR MARK)(2W)LA(W)MIXXIM(W)BB(W)100
                 OR TINOSORB(W)M OR TINUVIN(W)360 OR LA(W)31 OR JF(W)832
L26          1 S METHYLENEBIS(8W)TETRAMETHYLBUTYL(5W)(BENZOTRIAZOLYLPHENOL OR
                 BENZOTRIAZOL#)
L27          0 S METHYLENEBIS(3W)HYDROXY#(3W)BENZOTRIAZOL(4W)(TERT OR T)(2W)(OCTYLPHENYL
                 OR OCTYL(W)PHENYL)
L28          1 S METHYLENEBIS(8W)TETRAMETHYLBUTYL(5W)BENZOTRIAZOL?
L29          0 S BIS(3W)HYDROXY(3W)(TERT OR T)(2W)OCTYL(3W)BENZOTRIAZOL(5W)METHANE
L30          0 S METHYLENEBIS(3W)HYDROXY(3W)BENZOTRIAZOL(4W)(TERT OR T)(2W)(OCTYLPHENYL
                 OR OCTYL(W)PHENYL)
L31        189 S L24-L30
L32         38 S L31 AND (2010-2011)/PY
L33         28 DUP REM L32 (10 DUPLICATES REMOVED)
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L34           28 SORT L33 1-28 TI
                 SAVE L34 X0740BISOCT/A

L35           48 S 3846-71-7 OR EVERSORB(W)77 OR KEMISORB(W)75 OR SEESORB(W)705
                   OR SUMISORB(W) 320 OR TINUVIN(W) 320 OR VIOSORB(W) 582
L36           49 S HYDROXY(6W)(TERT OR T)(W)(BUTYLPHENYL OR BUTYL(W)PHENYL)(5W)
                   BENZOTRIAZOLE
L37           17 S (TERT OR T)(W)BUTYL(2W)HYDROXYPHENYL(5W)BENZOTRIAZOLE
L38            2 S (BENZOTRIAZOL OR BENZOTRIAZOLYL)(10W)(TERT OR T)(W)(BUTYLPHENOL OR
                   BUTYL(W)PHENOL)
L39            1 S PHENOL(5A)BENZOTRIAZOL(10W)(DIMETHYLETHYL OR (TERT OR T)(W)BUTYL
L40           93 S L35-L39
L41           15 S L40 AND (2010-2011)/PY
L42            6 DUP REM L41 (9 DUPLICATES REMOVED)
L43            6 SORT L42 1-6 TI
                 SAVE L43 X0740TIN320/A

L44          103 S 25973-55-1 OR (CHISORB OR UV OR TIN OR TINUVIN)(W)328
L45            0 S CYASORB(2W)2337 OR (EVERSORB OR UV OR KEMISORB)(W)74 OR LOWILITE
                   (W) 28 OR SEESORB(W) 704 OR SUMISORB(W) 350 OR VIOSORB(W) 591
L46            9 S HYDROXY(5W)(TERT OR T)(W)(AMYLPHENYL OR PENTYLPHENYL)(4W)BENZOTRIAZOLE
L47            3 S DI(2W)(TERT OR T)(W)(AMYL OR PENTYL)(2W)HYDROXYPHENYL(4W)BENZOTRIAZOLE
L48            5 S BENZOTRIAZOL(7W)DI(W)(TERT OR T)(W)(PENTYLPHENOL OR AMYLPHENOL)
L49            1 S BENZOTRIAZOL(10W)DIMETHYLPROPYL(5A)PHENOL
L50          106 S L44-L49
L51           43 S L50 AND (2010-2011)/PY
L52           26 DUP REM L51 (17 DUPLICATES REMOVED)
L53           26 SORT L52 1-26 TI
                 SAVE L53 X0740TIN328/A

L54            1 S 73936-91-1 OR CHISORB(W)5228 OR TINUVIN(W)928
L55            1 S (DIMETHYLBENZYL OR PHENYLETHYL)(10W)TETRAMETHYLBUTYL(2W)PHENYL
                (4W) BENZOTRIAZOLE OR TETRAMETHYLBUTYL(4W) BENZOTRIAZOL(4W) PHENOL
L56            8 S HYDROXY(8W)OCTYLPHENYL(4W)BENZOTRIAZOLE OR DIMETHYLBENZYL(4W)
                   (TERT OR T)(W) OCTYLPHENYL(4W) BENZOTRIAZOLE
L57            0 S PHENOL(4A)BENZOTRIAZOL(8W)METHYL(2W)PHENYLETHYL(8W)TETRAMETHY
L58           10 S L54-L56
L59            0 S L58 AND (2010-2011)
L60            6 DUP REM L58 (4 DUPLICATES REMOVED)
L61            6 SORT L60 1-6 TI
                 SAVE L61 X0740TIN928/A  [Redone on August 31, 2011]

L62           27 S 70321-86-7
L63          156 S BENZOTRIAZOLE(W)BT OR (EVERSORB OR LOWILITE OR T OR TINUVIN OR
                   UV)(W) 234# OR EVERSORB(W) 76 OR TINUVIN(W) 900 OR UVINUL(W)3034
L64            0 S BENZOTRIAZOLE(8W)BIS(5W)(DIMETHYLBENZYL(W)PHENOL OR
                   1(W)METHYL(W)1(W)PHENYLETHYL)
L65           14 S BENZOTRIAZOL(8W)BIS(5W)(DIMETHYL(W)PHENOL OR
                   1(W)METHYL(W)1(W)PHENYLETHYL)
L66            3 S HYDROXY(3W)BIS(5W)DIMETHYLBENZYL(W)PHENYL(4W)BENZOTRIAZOLE
L67            0 S DIMETHYLBENZYL(2W)HYDROXYPHENYL(W)BENZOTRIAZOLE
L68            0 S HYDROXY(8W)(CUMYLPHENYL OR CUMYL(W)PHENYL)(4W)BENZOTRIAZOLE
L69            0 S 1(W)METHYL(W)1(W)PHENYLETHYL(2W)HYDROXYPHENYL(W)BENZOTRIAZOLE
L70          172 S L62 OR L63 OR L65 OR L66
L71           60 S L70 AND (2010-2011)/PY
L72           24 DUP REM L71 (36 DUPLICATES REMOVED)
L73           24 SORT L72 1-24 TI
                 SAVE L73 X0740TIN900/A

L74           31 S 84268-33-7 OR TINUVIN(W)1130
L75            1 S BENZENEPROPANOIC(W)ACID(4A)BENZOTRIAZOL(8W)1(W)1(W)DIMETHYLETHYL
                  (3W)HYDROXY
L76            0 S (TERT OR T)(W)BUTYL(W)HYDROXY(10W)METHOXYCARBONYLETHYL(4W)BENZOTRIAZOLE
L78            2 S BENZOTRIAZOL(8W)4(W)HYDROXYPHENYL(2W)PROPIONATE
L79           33 S L74 OR L75 OR L78
L80            2 S L79 AND (2010-2011)/PY
L81            2 DUP REM L80 (0 DUPLICATES REMOVED)
L82            2 SORT L81 1-2 TI
                 SAVE L82 X740TIN1130/A
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L83         118 S 3864-99-1 OR (HISORP OR HISORB OR TINUVIN OR TNV OR UV)(W)327
L84         562 S CYASORB(2W)5357 OR EVERSORB(W)75 OR KEMISORB(W)72 OR LA(W)34 OR
                  LOWILITE(W)27 OR SEESORB(W) 702 OR UV(W) 2 OR UV(3W) 607 OR
                  VIOSORB(W) 580

L85          16 S L84 NOT UV(W)2
L86          16 S CYASORB(2W)5327 OR EVERSORB(W)75 OR KEMISORB(W)72 OR LA(W)34
                  LOWILITE(W)27 OR SEESORB(W)702 OR UV(3W)607 OR VIOSORB(W)580
L87          58 S HYDROXY(10W)(TERT OR T)(W)BUTYLPHENYL(4W)(CHLOROBENZOTRIAZOLE
                  OR CHLORO(4W)BENZOTRIAZOLE OR BENZOTRIAZOLE)
                  [This query and the next would have given some
                  non-chlorobenzotriazoles.]
L88          42 S DI(W)(TERT OR T)(W)BUTYL(3W)HYDROXYPHENYL(4W)(CHLOROBENZOTRIAZOLE
                  OR CHLORO(4W)BENZOTRIAZOLE OR BENZOTRIAZOLE)
L89           0 S CHLORO(4W)BENZOTRIAZOL(10W)DIMETHYLETHYL(5A)PHENOL
L90         758 S L83 OR L84 OR L86 OR L87 OR L88
L91         212 S L83 OR L86 OR L87 OR L88
L92          57 S L91 AND (2010-2011)/PY
L93          30 DUP REM L92 (27 DUPLICATES REMOVED)
L94          30 SORT L93 1-30 TI
                SAVE L94 X0740TIN327/A
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L16         929 3896-11-5 OR BUMETRIZOLE
L17          33 HYDROXY(3A)(TERT OR T)(W) BUTYL(5W)(CHLOROBENZOTRIAZOLE OR CHLORO(3W)
               BENZOTRIAZOLE OR CHLORO(3W) BENZO(2W) TRIAZOLE)
L18           0 (TERT OR T)(W) BUTYL(2W) METHYL(2W) HYDROXYPHENYL(2W) CHLOROBENZOTRIAZOLE
L19          11 ADK(W) STAB(W) LA(W) 36## OR BENAZOL(W) PBKH OR CIBATEX(W) LF
                OR (EVERSORB OR KEMISORB)(W) 73 OR J(W) 395
L20         139 JC(W) 30S OR JF(W) 79 OR LA(W) 36 OR LOWILITE(W) 26 OR SEESORB(W)
                (703 OR 300) OR (TIN OR TINUVIN OR TNV OR UV)(W) 326
L21         174 TINOGARD(W) AS OR TOMISORB(W) 600 OR (VIOSORB OR VS)(W) 550
L22        1208 (L16 OR L17 OR L18 OR L19 OR L20 OR L21)
L23         197 L22 AND (2010-2011)/PY
L24         197 SORT L23 TI
                SAVE L24 X0740BUMET/A

L25        5285 BENZOTRIAZOLE OR 95-14-7
L26         245 2H(W) BENZOTRIAZOLE
L27        2235 95-14-7 OR 1H(W) BENZOTRIAZOLE OR 1(W) 2(W) 3(W) BENZOTRIAZOLE
L28           0 1(W) 2(W) 3(W)(TRIAZA(W) 1H(W) INDENE OR TRIAZAINDENE) OR 1(W)
               2(W) AMINOAZOPHENYLENE
L29           1 2(W) 3(W) DIAZAINDOLE OR AZIMIDOBENZENE OR AZIMINOBENZENE OR
               B(W) 0094
L30          24 BENZENE(W) AZIMIDE OR BENZISOTRIAZOLE OR BLS(W) 1326 OR BT(W)
               120 OR COBRATEC(W)(35G OR 99)
L31          11 D(W) 32(W) 108 OR ENTEK OR IRGASTAB(W) I(W) 489 OR ISK(W) 3 OR
               KEMITEC(W) TT
L32          69 M(W) 318 OR NSC(W) 3058 OR RUSMIN(W) R OR SEETEC(W) BT? OR
               VERZO NE(W) CRYSTAL
L33        2329 (L27 OR L28 OR L29 OR L30 OR L31 OR L32)
L34         355 L33 AND (2010-2011)/PY
               SET DUPORDER FILE
L35         294 DUP REM L34 (61 DUPLICATES REMOVED)
L36         294 SORT L35 1-294 TI
                SAVE L36 X0740BZT/A
```

Session 3 to improve search on one compound (August 31, 2011)

```
L1            1 73936-91-1 OR TINUVIN(W) 928 OR CHISORB(W) 5228
L2            0 1(W) METHYL(W) 1(W) PHENYLETHYL(6W) TETRAMETHYLBUTYL(W) 6(W)
               BENZOTRIAZOL(W) 2(W) YL(W) PHENOL
L3            0 HYDROXY(3W) CUMYL(W) 5(W)(TERT OR T)(W) OCTYLPHENYL(3W) BENZOTRIAZOLE
L4            0 HYDROXY(5W) DIMETHYLBENZYL(7W) TETRAMETHYLBUTYL(W) PHENYL(W)
               BENZOTRIAZOLE
L5            0 HYDROXY(4W) DIMETHYLBENZYL(W) 5(W)(TERT OR T)(W) OCTYLPHENYL(3W)
                BENZOTRIAZOLE
L6            0 DIMETHYLBENZYL(2W) HYDROXY(6W) TETRAMETHYLBUTYL(W) PHENYL(3W)
               BENZOTRIAZOLE
```

The one record was a patent on a common application and was not saved.

<u>Set 2</u>

Set 2 contained benzotriazoles of potential interest that had been identified in 2010. No date limitations were placed on the results and the results for each set were combined into one to eliminate duplicates. Records were readily assigned to the appropriate group in EndNote by consulting the records in the MS Word file in which the keywords are boldfaced. The STN International databases were searched on September 1, 2011. The edited online history is reproduced below.

```
L1            0 S 127519-17-9
L2            0 S (BENZENEPROPANO? OR BENZENEPROPION?)(6A)HYDROXY(6A)BENZOTRIAZOL?(12A)
                  ESTERS

L5            3 S 84268-36-0
L8            0 S NAPHTHO(4W)TRIAZOL(W)2(W)YL(6W)TETRAMETHYLBUTYL(W)PHENOL
L9            0 S PHENOL(4W)NAPHTHO(4W)TRIAZOL(W)2(W)YL(6W)TETRAMETHYLBUTYL

L10           0 S 27876-55-7
L11           0 S HYDROXY(W)5(W)(TERT OR T)(W)OCTYLPHENYL(W)NAPHTHOTRIAZOLE
L12          11 S 3147-76-0 OR PHENOL(4W)BENZOTRIAZOL(W)2(W)YL(4W)DIMETHYLETHYL
L13           0 S BENZOTRIAZOL(W)2(W)YL(4W)(DIMETHYLETHYLPHENOL OR DIMETHYLETHYL
L15           2 S HYDROXY(W)5(W)(T OR TERT)(W)BUTYLPHENYL(3W)BENZOTRIAZOLE
L16           0 S BENZOTRIAZOL(W)2(W)YL(W)4(W)(TERT OR T)(W)(BUTYLPHENOL OR
                  BUTYL(W) PHENOL)
L17           4 S EVERSORB(W)70 OR (TINUVIN OR UV)(W)PS
L18          16 S L12-L17

L21           0 S 31701-42-5
L22           0 S NSC(W)375989
L23           0 S BENZOTRIAZOL(W)2(W)YL(3W)(BENZENEDIOL OR HYDROQUINONE)
L24           2 S (BENZENEDIOL OR HYDROQUINONE)(3W)BENZOTRIAZOL?
L59           5 S 3287-17-0 OR (TINUVIN OR UV)(W)301
L26           1 S CHLORO(3W)BENZOTRIAZOL(W)2(W)YL(4W)(DIMETHYLETHYL OR (TERT OR
                  T)(W) BUTYL)(W) PHENOL
L27          12 S (T OR TERT)(W)BUTYL(3W)CHLORO(3W)BENZOTRIAZOL(W)2(W)YL(W)PHENOL
L28           0 S HYDROXY(2W)(T OR TERT)(W)BUTYLPHENYL(2W)CHLOROBENZOTRIAZOLE
L29          18 S L59-L28

L32           3 S 36437-37-3 OR CHISORB(W)350 OR EVERSORB(W)79
L33           0 S BENZOTRIAZOL(W)2(W)YL(4W)(DIMETHYLETHYL OR (T OR TERT)(W)BUTYL
                  (3W)(METHYLPROPYL OR SEC(W) BUTYL)(W) PHENOL
L34           0 S HYDROXY(2W)SEC(W)BUTYL(2W)(T OR TERT)(W)BUTYLPHENYL(3W)BENZOTRIAZOLE
L35           0 S BENZOTRIAZOL(4W)(T OR TERT)(W)BUTYL(2W)SEC(W)(BUTYL(W)PHENOL
L36           0 S SEC(W)BUTYL(2W)(T OR TERT)(2W)HYDROXYPHENYL(W)BENZOTRIAZOLE
L37           0 S (T OR TERT)(W)BUTYL(2W)SEC(W)BUTYL(3W)BENZOTRIAZOL(3W)PHENOL
L38           3 S L32-L37

L41           2 S 83741-30-4 OR BENZOTRIAZOL(4W)(HYDROXYPHENYL(W)ETHANONE OR
                  HYDROXYPHENYLETHANONE)
L42           0 S ACETYL(4A)HYDROXYPHENYL(4A)BENZOTRIAZOL?
L43           0 S BENZOTRIAZOL?(6A)ACETYLPHENOL
L44           0 S BENZOTRIAZOL?(6A)HYDROXY(6A)ACETYLPHENYL

L46           2 S 84268-08-6 OR (TINUVIN OR UV)(W)840
L47           0 S (HEXANEDIOL OR HEXANEDIYL)(W)BIS(W)3(W)BENZOTRIAZOL(4W)(T OR
                  TERT)(W) BUTYL(2W) HYDROXYBENZENEPROPIONATE
L48           0 S (HEXANEDIYL OR HEXANEDIOL)(6A)BENZOTRIAZOL?(8W)PHENYLPROPRIONATE

L50          32 S 84268-33-7 OR (TINUVIN OR UV)(W)1130

L52           0 S 96549-95-0
L53           0 S JF(W)269
L54           0 S HYDROXY(3W)(HYDROXYETHYLPHENYL OR HYDROXYETHYL(W)PHENYL)(3W)
               BENZOTRIAZOLE
L55           0 S BENZENEETHANOL(4W)BENZOTRIAZOL(4W)HYDROXY
L56           0 S BENZOTRIAZOL(4W)(HYDROXY(W)BENZENEETHANOL OR HYDROXYBENZENEETHANOL
L57          68 S L5 OR L18 OR L29 OR L38 OR L41 OR L46 OR L50
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L58          61 DUP REM L57 (7 DUPLICATES REMOVED)
L59          61 SORT L58 1-61 TI
                SAVE L59 X0740SET2/A
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Set 3

Set 3 contained hydroxyphenylbenzotriazoles identified in 2011 that had no substitutions on the benzotriazole moiety. These compounds were selected from lists of hydroxyphenylbenzotriazoles found by Google searches. Again no date limitations were used in the STN searches. The online history of the September 8, 2011, search is reproduced below.

```
L1            3 84268-36-0
L2            0 3(W) 2H(W) BENZOTRIAZOL(W) 2(W) YL(W) 5(W) 1(W) 1(W) DIMETHYLETHYL
                (W) 4(W) HYDROXYBENZENEPROPIONIC(W) ACID
L3            0 3(W) 3(W) 2H(W) BENZOTRIAZOLYL(W) 2(W) YL(W) 5(W)(TERT OR T)(W)
                BUTYL(W) 4(W) HYDROXYPHENYL(W) PROPIONIC(W) ACID
L4            0 3(W) 2H(W) BENZOTRIAZOL(W) 2(W) YL(W) 5(W) 1(W) 1(W) DIMETHYLETH
                YL(W) 4(W) HYDROXYBENZENEPROPANOIC(W) ACID

L5           11 96478-09-0
L6            7 NORBLOC OR RUVA(W) 93 OR SOLTEX(W) EE
L7            0 TINUVIN(W) R796 OR TINUVIN(W) R(W) 796
L8            0 HYDROXY(3W)(METHACRYLOYLOXYETHYLPHENYL OR METHACRYLOYLOXYETHYL(W
                ) PHENYL)(3A) BENZOTRIAZOLE
L9           15 2(W) 3(W) 2H(W) BENZOTRIAZOL(W) 2(W) YL(W) 4(W) HYDROXYPHENYL(W)
                 ETHYL(W) METHACRYLATE
L10           0 4(W) 2(W) METHACRYLOYLOXYETHYL(W) 2(W) 2H(W) BENZOTRIAZOL(W)
                2(W) YL(W) PHENOL
L11          26 (L5 OR L6 OR L7 OR L8 OR L9 OR L10)

L12           2 83044-89-7
L13           2 (TINUVIN OR UV)(W) 109
L14           0 BENZENEPROPANOIC(W) ACID(W) 3(W) 5(W) CHLORO(W) 2H(W) BENZOTRIAZ
                OL(W) 2(W) YL(W) 5(W) 1(W) 1(W) DIMETHYLETHYL(W) 4(W) HYDROXY(W)
                 OCTYL(W) ESTER
L15           0 (TERT OR T)(W) BUTYL(3W) OCTYLOXYCARBONYLETHYL(2W) HYDROXYPHENYL
                (W) 5(W) CHLOROBENZOTRIAZOLE
L16           0 CHLORO(W) 2H(W) BENZOTRIAZOL(W) 2(W) YL(W) 5(W)(T OR TERT)(W)
                BUTYL(W) 4(W) HYDROXYPHENYL(W) PROPANOIC(W) OCTYL(W) ESTER
L17           0 OCTYL(W) 5(W)(T OR TERT)(W) BUTYL(W) 3(W) 5(W) CHLORO(W) 2H(W)
                BENZOTRIAZOL(W) 2(W) YL(W) 4(W) HYDROXYBENZENEPROPIONATE
L18           3 (L12 OR L13 OR L14 OR L15 OR L16 OR L17)

L19           2 10096-91-0
L20           2 L19 OR CGL(W) 900

L21           2 3147-77-1
L22           0 SEESORB(W) 707 OR SUMISORB(W)(310 OR 510) OR VIOSORB(W) 510
L23           1 HYDROXY(2W) OCTYLOXYPHENYL(3W) BENZOTRIAZOLE
L24           3 (L21 OR L22 OR L23)

L25           2 84268-23-5
L26           6 (TINUVIN OR UV)(W)(384 OR 99)
L27           0 BENZENEPROPANOIC(W) ACID(W) 3(W) 2H(W) BENZOTRIAZOL(W) 2(W) YL(W)
                5(W) 1(W) 1(W) DIMETHYLETHYL(W) 4(W) HYDROXY(W) OCTYL(W) ESTER
L28           0 (T OR TERT)(W) BUTYL(2W) HYDROXY(3W) OCTYLOXYCARBONYLETHYL(W)
                PHENYL(3W) BENZOTRIAZOLE
L29           0 2(W) 2(W) HYDROXY(W) 3(W)(T OR TERT)(W) BUTYL(W) 5(W) 2(W) OCTYL
                CARBONYLETHYL(W) PHENYL(3W) BENZOTRIAZOLE
L30           0 OCTYL(5W) BENZOTRIAZOL(W) 2(W) YL(W) 5(W)(T OR TERT)(W) BUTYL(W)
                 4(W)(HYDROXYHYDROCINNAMATE OR HYDROXYPHENYL(W) PROPIONATE)
L31           8 (L25 OR L26 OR L27 OR L28 OR L29 OR L30)
L32           6 L31 NOT BENZOTRIAZOL?
L33           5 L32 NOT UV(W) 384
L34           1 UV(W) 384
L35           7 L31 NOT UV(W) 384
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L36          11 23328-53-2
L37          13 TINOGARD(W) TL OR TINUVIN(W)(171 OR 571) OR UV(W) 571
L38           0 HYDROXY(5A) DODECYL(5A) METHYLPHENYL(3W) BENZOTRIAZOLE
L39           0 2(W) 2H(W) BENZOTRIAZOL(W) 2(W) YL(W) 6(W) DODECYL(W)(4(W) METHY
                LPHENOL OR P(W) CRESOL)
L40          17 (L36 OR L37 OR L38 OR L39)

L41           2 136457-10-8
L42          32 (TINUVIN OR T)(W) 213
L43          26 T(W) 213
L44           6 L41 OR TINUVIN(W) 213
L45           9 UV(W) 213
L46           0 POLYETHYLENE(W) GLYCOL(W) MONO(W) 2(W) 2(W) 2H(W) BENZOTRIZOL(W)
                 2(W) YL(W) 6(W)(T OR TERT)(W) 4(W) 3(W) METHOXY(W) 3(W) OXYPROP
                YL(W) PHENYL(W) ETHER

L47           7 104810-47-1

L48          13 104810-48-2
L49          24 (TINUVIN OR TV)(W) 1130
L50          27 L48 OR L49
L51          85 L1 OR L11 OR L18 OR L24 OR L35 OR L40 OR L44 OR L47 OR L50
                SET DUPORDER FILE
L52          68 DUP REM L51 (17 DUPLICATES REMOVED)
                 ANSWERS '1-4' FROM FILE MEDLINE
                 ANSWERS '5-6' FROM FILE AGRICOLA
                 ANSWERS '7-14' FROM FILE CABA
                 ANSWERS '15-16' FROM FILE BIOSIS
                 ANSWERS '17-65' FROM FILE TOXCENTER
                 ANSWER '66' FROM FILE FSTA
                 ANSWERS '67-68' FROM FILE EMBASE
                SAVE L51 X0740SET3NOM/Q
L53          68 SORT L52 1-68 TI
                SAVE L53 X0740SET3BIO/A
```

Searches for two additional compounds were done on September 20, 2011. The compound with CAS RN 207738-63-4 had been inadvertantly omitted from the Set 1 searches. The compound with CAS RN 2170-39-0 had been found in three references during extraction of data for other benzotriazoles. The usual databases were used. The online strategy follows:

```
L1            0 S 207738-63-4
L2            0 S 2(W)1(W)METHYL(W)1(W)PHENYLETHYL(W)4(W)1(W)1(W)1(W)3(W)TETRAMETHYLBUTYL
                (W)6(W)5(W)TRIFLUOROMETHYL(3A)BENZOTRIAZOL(W)2(W)YL(W)PHENOL
L3            0 S 2(W)1(W)METHYL(W)PHENYLETHYL(W)4(W)1(W)1(W)1(W)3(W)TETRAMETHYLBUTYL
                (W)6(W)5(W)TRIFLUOROMETHYLBENZOTRIAZOL(W)2(W)YL(W)PHENOL
L4            0 S 2(W)3(W).ALPHA.(W)CUMYL(W)2(W)HYDROXY(W)5(W)(T OR
                TERT)(W)OCYLPHENYL(W)5(W)TRIFLUOROMETHYL(W)2H(W)BENZOTRIAZOLE
L5            0 S 5(W)TRIFLUOROMETHYL(W)2(W)2(W)HYDROXY(W)3(W).ALPHA.(W)CUMYL(W)5(W)(TERT
                OR T)(W)OCTYLPHENYL(W)2H(W)BENZOTRIAZOLE
L6            7 S 2170-39-0
L7            0 S PHENOL(W)2(W)2H(W)BENZOTRIAZOL(W)2(W)YL(W)4(W)METHYL(W)6(W)2(W)
                PROPEN(W)1(W)YL
L8            0 S 2(W)2H(W)BENZOTRIAZOL(W)2(W)YL(W)4(W)METHYL(W)6(W)2(W)PROPEN(W)
                1(W)YLPHENOL
L9            0 S PHENOL(W)2(W)2H(W)BENZOTRIAZOL(W)2(W)YL(W)4(W)METHYL(W)6(W)2(W)PROPENYL
L10           0 S 2(W)2H(W)BENZOTRIAZOL(W)2(W)YL(W)4(W)METHYL(W)6(W)2(W)PROPENYLPHENOL
L11           0 S P(W)CRESOL(W)2(W)ALLYL(W)6(W)2H(W)BENZOTRIAZOL(W)2(W)YL
L12           0 S 2(W)ALLYL(W)6(W)2H(W)BENZOTRIAZOL(W)2(W)YL(W)P(W)CRESOL
L13           1 S ALLYL(3A)HYDROXY(3A)METHYLPHENYL(W)BENZOTRIAZOLE
L14           7 S L6-L13
                SET DUPORDER FILE
L15           7 DUP REM L14 (0 DUPLICATES REMOVED) [All records were in TOXCENTER.]
L16           7 SORT L15 1-7 TI
                SAVE L16 X0740MOREBIO/A
```

No results were found for 207738-63-4. Six of the 7 records for 2170-39-0 were of interest, three of which were new.

Registry searches for Sets 1 and 2 had been done on August 17, 2010. Registry searches for Set 3 were done on September 2, 2011. RTECS searches for the various sets were done on August 17 and 19, 2010. CAPLUS searches for occurrence of the compounds as pollutants were done on August 23, 2010, and September 7 and 23, 2011. Google and Google Scholar were used as needed to fill information gaps.

Appendix C. Synonyms for Phenolic Benzotriazoles
[in order of appearance in report]

CASRN	Chemical (CA Index) Name	Synonyms
10096-91-0	Phenol, 2-(2H-benzotriazol-2-yl)-	Phenol, o-2H-benzotriazol-2-yl- (7CI, 8CI) 2-(2'-Hydroxyphenyl)-2H-benzotriazole 2-(2'-Hydroxyphenyl)benzotriazole 2-(2-Hydroxyphenyl)benzotriazole 2-(2H-Benzotriazol-2-yl)phenol 2-(o-Hydroxyphenyl)-2H-benzotriazole 2-(o-Hydroxyphenyl)benzotriazole CGL 900
2440-22-4	Phenol, 2-(2H-benzotriazol-2-yl)-4-methyl-	p-Cresol, 2-(2H-benzotriazol-2-yl)- 2-(2'-Hydroxy-5'-methylphenyl)benzotriazole 2-(2-Hydroxy-5-methyl)benzotriazole 2-(2-Hydroxy-5-methylphenyl)-2H-benzotriazole 2-(2-Hydroxy-5-methylphenyl)benzotriazole 2-(2H-Benzotriazol-2-yl)-4-methylphenol 2-(2H-Benzotriazol-2-yl)-p-cresol 2-(5'-Methyl-2'-hydroxyphenyl)benzotriazole 2-(5-Methyl-2-hydroxyphenyl)benzotriazole 2-Benzotriazol-2-yl-4-methylphenol ADK Stab LA 32 ADK-ARKLS DN 13 Benazol II Benazol P BT 1 BT 1 (light stabilizer) Dainsorb T 1 Drometrizole Eversorb 71 JF 77 JF 77P JF 77T Kemisorb 71 LA 32 Lowilite 55 Mark LA 32 NSC 91885 Seesorb 701 Seikalizer AZ Sumisorb 200 Tinuvin P UV Absorber 1 UV-P UV-P (UV stabilizer) UVA-P Uvasorb SV Uvinul 3033P Viosorb 520
3147-76-0	Phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1-dimethylethyl)-	Phenol, 2-(2H-benzotriazol-2-yl)-4-tert-butyl- (7CI, 8CI) 2-(2'-Hydroxy-5'-tert-butylphenyl)benzotriazole 2-(2-Hydroxy-5-tert-butyl)benzotriazole 2-(2-Hydroxy-5-tert-butylphenyl)-2H-benzotriazole 2-(2-Hydroxy-5-tert-butylphenyl)benzotriazole 2-(2H-Benzotriazol-2-yl)-4-tert-butyl-phenol 2-(5'-tert-Butyl-2'-hydroxyphenyl)benzotriazole 2-(5-tert-Butyl-2-hydroxyphenyl)benzotriazole Eversorb 70 Tinuvin PS
3287-17-0	Phenol, 2-(5-chloro-2H-benzotriazol-2-yl)-4-(1,1-dimethylethyl)-	Phenol, 4-tert-butyl-2-(5-chloro-2H-benzotriazol-2-yl)- 2-(2'-Hydroxy-5'-tert-butylphenyl)-5-chlorobenzotriazole Tinuvin 301

CASRN	Chemical (CA Index) Name	Synonyms
3147-75-9	Phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)-	2-[2'-Hydroxy-5'-(1,1,3,3-tetramethylbutyl)phenyl]benzotriazole 2-(2-Hydroxy-5-tert-octylphenyl)benzotriazole 2-(2-Hydroxy-5-tert-octylphenyl)-2H-benzotriazole 2-(2'-Hydroxy-5'-tert-octylphenyl)benzotriazole 2-(2'-Hydroxy-5'-tert-octylphenyl)benztriazole 2-(2-Hydroxy-5-t-octylphenyl)-2H-benzotriazole 2-(2-Hydroxy-5-t-octylphenyl)benzotriazole 2-(2'-Hydroxy-5'-t-octylphenyl)benzotriazole 2-(5-t-Octyl-2-hydroxyphenyl)benzotriazole 2-Benzotriazolyl-4-tert-octylphenol Benzotriazole Anti UV 5411 Chisorb 5411 Cyasorb 5411 Cyasorb UV 5411 Eversorb 72 JF 83 Kemisorb 79 Octrizole Seesorb 709 Spectra-Sorb UV 5411 Sumisorb 340 Tinuvin 329 UV 329 UV 5411 Uvinul 3029 Viosorb 583
96549-95-0	Benzeneethanol, 3-(2H-benzotriazol-2-yl)-4-hydroxy-	2-(2'-Hydroxy-5'-(2-hydroxyethyl)phenyl)benzotriazole 2-[2'-Hydroxy-5'-(2-hydroxyethyl)phenyl]-2H-benzotriazole 2-[2-Hydroxy-5-(2-hydroxyethylphenyl)]-2H-benzotriazole JF 269
83741-30-4	Ethanone, 1-[3-(2H-benzotriazol-2-yl)-4-hydroxyphenyl]-	
96478-09-0	2-Propenoic acid, 2-methyl-, 2-[3-(2H-benzotriazol-2-yl)-4-hydroxyphenyl]ethyl ester	2-(2'-Hydroxy-5'-(2-methacryloyloxyethyl)phenyl)benzotriazole 2-(2'-Hydroxy-5'-methacryloxyethylphenyl)-2H-benzotriazole 2-(2'-Hydroxy-5'-methacryoxyethylphenyl)-2H-benzotriazole 2-[2-Hydroxy-5-(2-methacryloyloxyethyl)phenyl]-2H-benzotriazole 2-[3-(2H-Benzotriazol-2-yl)-4-hydroxyphenyl]ethyl methacrylate 4-(2-Methacryloyloxyethyl)-2-(2H-benzotriazol-2-yl)phenol Norbloc Norbloc 7966 RUVA 93 Soltex EE
2170-39-0	Phenol, 2-(2H-benzotriazol-2-yl)-4-methyl-6-(2-propen-1-yl)-	p-Cresol, 2-allyl-6-(2H-benzotriazol-2-yl)- (7CI, 8CI) Phenol, 2-(2H-benzotriazol-2-yl)-4-methyl-6-(2-propenyl)- (9CI) 2-(3'-Allyl-2'-hydroxy-5'-methylphenyl)benzotriazole
23328-53-2	Phenol, 2-(2H-benzotriazol-2-yl)-6-dodecyl-4-methyl-	p-Cresol, 2-(2H-benzotriazol-2-yl)-6-dodecyl- (8CI) (2-Hydroxy-3-dodecyl-5-methylphenyl)benzotriazole 2-(2-Hydroxy-3-dodecyl-5-methylphenyl)-2H-benzotriazole 2-(2-Hydroxy-3-dodecyl-5-methylphenyl)benzotriazole 2-(2H-Benzotriazol-2-yl)-6-dodecyl-4-methylphenol 2-(3'-Dodecyl-2'-hydroxy-5'-methylphenyl)benzotriazole 2-(3'-Dodecyl-5'-methyl-2'-hydroxyphenyl)benzotriazole 2-(3-Dodecyl-2-hydroxy-5-methylphenyl)benzotriazole 2-(Benzotriazol-2-yl)-6-dodecyl-4-methylphenol Tinogard TL Tinuvin 171 Tinuvin 571 UV 571
36437-37-3	Phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1-dimethylethyl)-6-(1-methylpropyl)-	2-(2-Hydroxy-3-sec-butyl-5-tert-butylphenyl)benzotriazole 2-(2-Hydroxy-3-sec-butyl-5-tert-butylphenyl)-2H-benzotriazole 2-(2H-Benzotriazol-2-yl)-4-(tert-butyl)-6-(sec-butyl)phenol 2-(3'-sec-Butyl-5'-tert-butyl-2'-hydroxyphenyl)benzotriazole 2-(3-sec-Butyl-5-tert-butyl-2-hydroxyphenyl)benzotriazole 4-tert-Butyl-6-sec-butyl-2-(2H-benzotriazol-2-yl)phenol Chisorb 350 Eversorb 79 Tinuvin 350†

CASRN	Chemical (CA Index) Name	Synonyms
3896-11-5	Phenol, 2-(5-chloro-2H-benzotriazol-2-yl)-6-(1,1-dimethylethyl)-4-methyl-	p-Cresol, 2-tert-butyl-6-(5-chloro-2H-benzotriazol-2-yl)- (7CI, 8CI) 2-(2'-Hydroxy-3'-tert-butyl-5'-methylphenyl)-5-chlorobenzotriazole 2-(2'-Hydroxy-3'-tert-butyl-5'-methylphenyl)-5-chlorobenztriazole 2-(2'-Hydroxy-3'-tert-butyl-5-methylphenyl)-5-chlorobenzotriazole 2-(2-Hydroxy-3-tert-butyl-5-methylphenyl)-5-chloro-2H-benzotriazole 2-(2-Hydroxy-3-tert-butyl-5-methylphenyl)-5-chlorobenzotriazole 2-(3'-tert-Butyl-2'-hydroxy-5'-methylphenyl)-5-chlorobenzotriazole 2-(3'-tert-Butyl-5'-methyl-2'-hydroxyphenyl)-5-chlorobenzotriazole 2-(3-tert-Butyl-2-hydroxy-5-methylphenyl)-5-chloro-2H-benzo-v-triazole 2-(3-tert-Butyl-2-hydroxy-5-methylphenyl)-5-chlorobenzotriazole 2-(3-tert-Butyl-5-methyl-2-hydroxyphenyl)-5-chlorobenzotriazole 2-(5-Chloro-2H-benzotriazol-2-yl)-6-(1,1-dimethylethyl)-4-methylphenol 2-tert-Butyl-6-(5-chloro-2-benzotriazolyl)-4-methylphenol 2-tert-Butyl-6-(5-chloro-2H-benzotriazol-2-yl)-4-methylphenol 2-[5-Chloro-2H-benzotriazol-2-yl]-4-methyl-6-(tert-butyl)phenol 5-Chloro-2-(2-hydroxy-3-tert-butyl-5-methylphenyl)-2H-benzotriazole 5-Chloro-2-(3-tert-butyl-2-hydroxy-5-methylphenyl)benzotriazole A-Light ADK Stab LA 36 ADK Stab LA 36RG Benazol PBKh Bumetrizole Cibatex LF Eversorb 73 J 395 J 395 (light stabilizer) JC 30S JF 79 Kemisorb 73 LA 36 Lowilite 26 Mark LA 36 Seesorb 703 Sumisorb 300 Tin 326 Tinogard AS Tinuvin 326 TNV 326 Tomisorb 600 UV 326 Viosorb 550 VS 550
3846-71-7	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-di-tert-butyl- (7CI, 8CI) 2-(2'-Hydroxy-3',5'-di-t-butylphenyl)benzotriazole 2-(2'-Hydroxy-3',5'-di-tert-butylphenyl)benzotriazole 2-(2'-Hydroxy-3'5-di-tert-butylphenyl) benzotriazole 2-(2-Benzotriazolyl)-4,6-di-tert-butylphenol 2-(2-Hydroxy-3,5-di-tert-butylphenyl)-2H-benzotriazole 2-(2-Hydroxy-3,5-di-tert-butylphenyl)benzotriazole 2-(3',5'-Di-tert-butyl-2'-hydroxyphenyl)benzotriazole 2-(3,5-Di-tert-butyl-2-hydroxyphenyl)-2H-benzotriazole 2-(3,5-Di-tert-butyl-2-hydroxyphenyl)benzotriazole 2-Benzotriazol-2-yl-4,6-di-tert-butylphenol** Benzotriazol-2-yl-4,6-di-tert-butyl-phenol Eversorb 77 Kemisorb 75 Seesorb 705 Sumisorb 320 Tinuvin 320 Viosorb 582

CASRN	Chemical (CA Index) Name	Synonyms
3864-99-1	Phenol, 2-(5-chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-	Phenol, 2,4-di-tert-butyl-6-(5-chloro-2H-benzotriazol-2-yl)- (7CI, 8CI) 2,4-Di-tert-butyl-6-(5-chloro-2H-benzotriazol-2-yl)phenol 2,4-Di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol 2-(2'-Hydroxy-3',5'-di-tert-butylphenyl)-5-chlorobenzotriazole 2-(2-Hydroxy-3,5-di-tert-butylphenyl)-5-chloro-2H-benzotriazole 2-(2-Hydroxy-3,5-di-tert-butylphenyl)-5-chlorobenzotriazole 2-(3',5'-Di-tert-butyl-2'-hydroxyphenyl)-5-chlorobenzotriazole 2-(3,5-Di-tert-butyl-2-hydroxyphenyl)-5-chloro-2H-benzotriazole 2-(3,5-Di-tert-butyl-2-hydroxyphenyl)-5-chlorobenzotriazole 5-Chloro-2-(2-hydroxy-3,5-di-tert-butylphenyl)-2H-benzotriazole 5-Chloro-2-(2-hydroxy-3,5-di-tert-butylphenyl)benzotriazole 5-Chloro-2-(3',5'-di-tert-butyl-2'-hydroxyphenyl)benzotriazole 5-Chloro-2-(3,5-di-tert-butyl-2-hydroxyphenyl)-2H-benzotriazole 5-Chloro-2-(3,5-di-tert-butyl-2-hydroxyphenyl)benzotriazole ADK Stab LA 34 Cyasorb UV 5357 Eversorb 75 Hisorb 327 Hisorp 327 Kemisorb 72 LA 34 Lowilite 27 Mark LA 34 Seesorb 702 Tinuvin 327 TNV 327 UV 2 UV 2 (UV stabilizer) UV 327 UV-Chek AM 607 Viosorb 580
25973-55-1	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)-	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-di-tert-pentyl- (7CI, 8CI) 2-(2'-Hydroxy-3',5'-di-tert-amylphenyl)benzotriazole 2-(2-Hydroxy-3,5-di-tert-amylphenyl)-2H-benzotriazole 2-(2-Hydroxy-3,5-di-tert-amylphenyl)benzotriazole 2-(2-Hydroxy-3,5-di-tert-pentylphenyl)benzotriazole 2-(2H-Benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)phenol 2-(2H-Benzotriazol-2-yl)-4,6-di-tert-pentylphenol 2-(3',5'-Di-tert-amyl-2'-hydroxyphenyl)benzotriazole 2-(3,5-Di-tert-amyl-2-hydroxyphenyl)-2H-benzotriazole 2-(3,5-Di-tert-amyl-2-hydroxyphenyl)benzotriazole 2-(3,5-Di-tert-pentyl-2-hydroxyphenyl)-2H-benzotriazole 2-(3,5-Di-tert-pentyl-2-hydroxyphenyl)benzotriazole Chisorb 328 Cyasorb UV 2337 Eversorb 74 Kemisorb 74 Lowilite 28 Seesorb 704 Sumisorb 350 Tin 328 Tinuvin 328 UV 328 UV 74 Viosorb 591
70693-49-1	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1,3,3-tetramethylbutyl)-	2-(Benzotriazol-2-yl)-4,6-bis(2,4,4-trimethylpentan-2-yl)phenol* 2-(2-Hydroxy-3,5-bis(*tert*-octyl)phenyl)benzotriazole**
73936-91-1	Phenol, 2-(2H-benzotriazol-2-yl)-6-(1-methyl-1-phenylethyl)-4-(1,1,3,3-tetramethylbutyl)-	2-(1-Methyl-1-phenylethyl)-4-(1,1,3,3-tetramethylbutyl)-6-(benzotriazol-2-yl)phenol 2-(2-Hydroxy-3-α-cumyl-5-tert-octylphenyl)-2H-benzotriazole 2-[2'-Hydroxy-3'-(α,α-dimethylbenzyl)-5'-(1,1,3,3-tetramethylbutyl)phenyl]benzotriazole 2-[2-Hydroxy-3-(α,α-dimethylbenzyl)-5-tert-octylphenyl]-2H-benzotriazole 2-[3-(α,α-Dimethylbenzyl)-2-hydroxy-5-(1,1,3,3-tetramethylbutyl)phenyl]-2H-benzotriazole Chisorb 5228 Tinuvin 928

CASRN	Chemical (CA Index) Name	Synonyms
207738-63-4	Phenol, 2-(1-methyl-1-phenylethyl)-4-(1,1,3,3-tetramethylbutyl)-6-[5-(trifluoromethyl)-2H-benzotriazol-2-yl]-	2-(1-Methyl-1-phenylethyl)-4-(1,1,3,3-tetramethylbutyl)-6-(5-trifluoromethyl benzotriazol-2-yl)phenol 2-(3-α-Cumyl-2-hydroxy-5-tert-octylphenyl)-5-trifluoromethyl-2H-benzotriazole 5-Trifluoromethyl-2-[2-hydroxy-3-α-cumyl-5-tert-octylphenyl]-2H-benzotriazole CGL 139
70321-86-7	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)-	2-(2-Hydroxy-3,5-di-α-cumylphenyl)-2H-benzotriazole 2-(2H-Benzotriazol-2-yl)-4,6-bis(α,α-dimethylbenzyl)phenol 2-(2H-Benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol 2-(2H-Benzotriazol-2-yl)-4,6-bis(1-methyl-l-phenylethyl)phenol 2-(3',5'-Bis(α,α-dimethylbenzyl)-2'-hydroxyphenyl)benzotriazole 2-[2'-Hydroxy-3',5'-bis(α,α-dimethylbenzyl)phenyl]benzotriazole 2-[2-Hydroxy-3,5-bis(α,α-dimethylbenzyl)phenyl]-2H-benzotriazole 2-[2-Hydroxy-3,5-bis(α,α-dimethylbenzyl)phenyl]benzotriazole 2-[2-Hydroxy-3,5-di(α,α-dimethylbenzyl)phenyl]-2H-benzotriazole 2-[2-Hydroxy-3,5-di(1,1-dimethylbenzyl)phenyl]-2H-benzotriazole 2-[3',5'-Bis(1-methyl-1-phenylethyl)-2'-hydroxyphenyl]benzotriazole Benzotriazole BT Eversorb 234 Eversorb 76 Lowilite 234 T 234 Tinuvin 234 Tinuvin 234D Tinuvin 900 UV 234 UV 234 (antioxidant) Uvinul 3034
84268-36-0	Benzenepropanoic acid, 3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-	3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid 3-[3-(2H-Benzotriazol-2-yl)-5-tert-butyl-4-hydroxyphenyl]propionic acid
84268-33-7	Benzenepropanoic acid, 3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-, methyl ester	2-[3'-tert-Butyl-2'-hydroxy-5'-(2-methoxycarbonylethyl)phenyl]benzotriazole 3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-benzenepropanoic acid methyl ester Methyl 3-[3-tert-butyl-5-(2H-benzotriazol-2-yl)-4-hydroxyphenyl]propionate Tinuvin 1130**†
84268-08-6	Benzenepropanoic acid, 3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-, 1,1'-(1,6-hexanediyl) ester	Benzenepropanoic acid, 3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-, 1,6-hexanediyl ester (9CI) 1,6-Hexanediol bis(3-benzotriazol-2-yl-5-tert-butyl-4-hydroxybenzenepropionate) 1,6-Hexanediyl bis(3-benzotriazol-2-yl)-4-hydroxy-5-tert-butyl)phenylpropionate Tinuvin 840
84268-23-5	Benzenepropanoic acid, 3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-, octyl ester	2-(3'-tert-Butyl-2'-hydroxy-5'-(2-octyloxycarbonylethyl)phenyl)benzotriazole 2-[2-Hydroxy-3-tert-butyl-5-(2-octyloxycarbonylethyl)phenyl]-2H-benzotriazole 2-[3-tert-Butyl-2-hydroxy-5-(2-octyloxycarbonylethyl)phenyl]-2H-benzotriazole Octyl 3-(2H-benzotriazol-2-yl)-5-tert-butyl-4-hydroxyhydrocinnamate Octyl 3-(benzotriazol-2-yl)-5-tert-butyl-4-hydroxyhydrocinnamate Octyl 3-[3-(2H-benzotriazol-2-yl)-5-tert-butyl-4-hydroxyphenyl]propionate Tinuvin 384 Tinuvin 99 Tinuvin 99/2
83044-89-7	Benzenepropanoic acid, 3-(5-chloro-2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-, octyl ester	2-(3'-tert-Butyl-5'-(2-octyloxycarbonylethyl)-2'-hydroxyphenyl)-5-chlorobenzotriazole 3-[3-(5-Chloro-2H-benzotriazole-2-yl)-5-tert-butyl-4-hydroxyphenyl]propanoic acid octyl ester Octyl 5-tert-butyl-3-(5-chloro-2H-benzotriazole-2-yl)-4-hydroxybenzenepropionate Tinuvin 109
127519-17-9	Benzenepropanoic acid, 3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-, C7-9-branched and linear alkyl esters	4-Methylhexyl 3-[3-(benzotriazol-2-yl)-5-*tert*-butyl-4-hydroxyphenyl]propanoate* Tinuvin 384‡

CASRN	Chemical (CA Index) Name	Synonyms
103597-45-1	Phenol, 2,2'-methylenebis[6-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)-	2,2'-Methylenebis[4-(1,1,3,3-tetramethylbutyl)-6-(2H-benzotriazol-2-yl)phenol] 2,2'-Methylenebis[4-(1,1,3,3-tetramethylbutyl)-6-benzotriazol-2-ylphenol] 2,2'-Methylenebis[4-(1,1,3,3-tetramethylbutyl)-6-benzotriazolylphenol] 2,2'-Methylenebis[6-(2-benzotriazolyl)-4-(1,1,3,3-tetramethylbutyl)phenol] 2,2'-Methylenebis[6-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol] 2,2'-Methylenebis[6-(2H-benzotriazole-2-yl)-4-(1,1,3,3-tetramethylbutyl)]phenol Adekastab LA 31 ADK Stab LA 31 Bisoctrizole Bisoctyltriazole Bis[2-hydroxy-5-tert-octyl-3-(benzotriazol-2-yl)phenyl]methane Eversorb 78 FAT 75'634 JF 832 LA 31 Mark LA 31 MBBT Methylenebis(2-hydroxy-3-(benzotriazol-2-yl)-5-tert-octylphenyl) Mixxim ADK LA 31 Mixxim BB 100 Tinosorb M Tinuvin 360
27876-55-7	Phenol, 2-(2H-naphtho[1,2-d]triazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)-	2-(2'-Hydroxy-5'-t-octylphenyl)naphthotriazole
3147-77-1	Phenol, 2-(2H-benzotriazol-2-yl)-5-(octyloxy)-	2-(2'-Hydroxy-4'-octyloxyphenyl)benzotriazole 2-(2-Hydroxy-4-octyloxyphenyl)-2H-benzotriazole Seesorb 707 Sumisorb 310 Sumisorb 510 Viosorb 510
104810-48-2	Poly(oxy-1,2-ethanediyl), α-[3-[3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropyl]-Ω-hydroxy-	α-[3-[3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropyl]-Ω-hydroxypoly(oxy-1,2-ethanediyl) Tinuvin 1130† TV 1130
104810-47-1‡	Poly(oxy-1,2-ethanediyl), α-[3-[3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropyl]-Ω-[3-[3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy]-	α-3-[3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropyl-Ω-[3-[3-(2H-benzotriazol-2-yl)-5-1,1-dimethylethyl]-4-hydroxyphenyl]-1-oxopropylpoly(oxy-1,2-ethanediyl) α-[3-[3-(2H-Benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropyl]-Ω-[3-[3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy]poly(oxy-1,2-ethanediyl)

Primary Source: Registry (2010-2011)
Secondary Sources: When no synonyms were provided in the Registry record, any available from the *PubChem and/or **ChemIDplus record were reported.
Tertiary Sources: †Chemical Book (2008a); Tetrahedron (2010); ‡Chemical Book (2008b); NICNAS (1993)

†According to Registry, this CASRN is associated with the trade name Tinuvin 1130. In contrast, ChemIDplus associates the trade name with CASRN 84268-33-7 (i.e., BZT-Pr acid, ME). ‡Internet searches show that the trade name is also associated with CASRN 104810-47-1 or with both (i.e., 104810-47-1 and 104810-48-2] (e.g., chemBlink, 2011; Chemical Book, 2008; and ChemNet, undated).

Appendix D: Environmental Occurrence of Selected Phenolic Benzotriazoles

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
ditPe-BZT	25973-55-1	Blubbers of 5 finless porpoises	Japan, western, Ariake Sea regions	11-64 ng/g wet wt. (ppb)	Accidental catches of 2 females from 1999, 1 male in 2008, and a male and a female in 2009. Highest value in 1999.	Nakata et al. (2010 [PMID:20959922])
ditBu-BZT	3846-71-7	Blubbers of 5 finless porpoises	Japan, western, Ariake Sea regions	<0.05 ng/g wet wt. (ppb)	Accidental catches of 2 females from 1999, 1 male in 2008, and a male and a female in 2009.	Nakata et al. (2010 [PMID:20959922])
ditBu-ClBZT	3864-99-1	Blubbers of 5 finless porpoises	Japan, western, Ariake Sea regions	4.5-31 ng/g wet wt. (ppb)	Accidental catches of 2 females from 1999, 1 male in 2008, and a male and a female in 2009. Highest value in 2009.	Nakata et al. (2010 [PMID:20959922])
ditBu-BZT	3846-71-7	Bottom ash	Japan, pilot-scale incinerator	0.52 µg/kg	Amount: 0.419 µg	Watanabe and Noma (2010 [PMID:20227827])
ditBu-ClBZT	3864-99-1	Bottom ash	Japan, pilot-scale incinerator	0.063 µg/kg	Amount: 0.0507 µg	Watanabe and Noma (2010 [PMID:20227827])
Allyl-BZT	2170-39-0	Fish, muscle tissue of 20 spp.	Manila Bay, Philippines	Range of means/single values ND-5.40 ng/g lipid weight	A total of 58 specimens tested.	Kim et al. (2011, in press [PMID:21741069])
Drometrizole	2440-22-4	Fish, muscle tissue of 20 spp.	Manila Bay, Philippines	Range of means/single values 3.02-160 ng/g lipid weight	A total of 58 specimens tested.	Kim et al. (2011, in press [PMID:21741069])
ditPe-BZT	25973-55-1	Fish, muscle tissue of 20 spp.	Manila Bay, Philippines	Range of means/single values ND-207 ng/g lipid weight	A total of 58 specimens tested.	Kim et al. (2011, in press [PMID:21741069])
Octrizole	3147-75-9	Fish, muscle tissue of 20 spp.	Manila Bay, Philippines	Range of means/single values ND-39.4 ng/g lipid weight	A total of 58 specimens tested.	Kim et al. (2011, in press [PMID:21741069])
ditBu-BZT	3846-71-7	Fish, muscle tissue of 20 spp.	Manila Bay, Philippines	Range of means/single values 0.02-22.5 ng/g lipid weight	A total of 58 specimens tested.	Kim et al. (2011, in press [PMID:21741069])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
ditBu-ClBZT	3864-99-1	Fish, muscle tissue of 20 spp.	Manila Bay, Philippines	Range of means/single values ND-109 ng/g lipid weight	A total of 58 specimens tested.	Kim et al. (2011, in press [PMID:21741069])
Bumetrizole	3896-11-5	Fish, muscle tissue of 20 spp.	Manila Bay, Philippines	Range of means/single values ND-40.7 ng/g lipid weight	A total of 58 specimens tested.	Kim et al. (2011, in press [PMID:21741069])
diMeEtPh-BZT	70321-86-7	Fish, muscle tissue of 20 spp.	Manila Bay, Philippines	Range of means/single values ND-62.9 ng/g lipid weight	A total of 58 specimens tested.	Kim et al. (2011, in press [PMID:21741069])
Allyl-BZT	2170-39-0	Fish, muscle tissue of 3 spp.	Manila Bay, Philippines	ND to less than the method detection limit	The species were bluetail mullet (*Valamugil buchanani*, *n*=1), coral grouper (*Epinephelus corallicola, n*=1), and flathead gray mullet (*Mugil cephalus*, *n*=3).	Kim et al. (2011 [PMID:21531423])
Drometrizole	2440-22-4	Fish, muscle tissue of 3 spp.	Manila Bay, Philippines	Range of means/single values 9.07-160 ng/g lipid wt.	The species were bluetail mullet, *n*=1, coral grouper, *n*=1, and flathead gray mullet, *n*=3.	Kim et al. (2011 [PMID:21531423])
ditPe-BZT	25973-55-1	Fish, muscle tissue of 3 spp.	Manila Bay, Philippines	Range of means/single values 18.4-105 ng/g lipid wt.	The species were bluetail mullet, *n*=1, coral grouper, *n*=1, and flathead gray mullet, *n*=3.	Kim et al. (2011 [PMID:21531423])
Octrizole	3147-75-9	Fish, muscle tissue of 3 spp.	Manila Bay, Philippines	Range of means/single values ND-39.4 ng/g lipid wt.	The species were bluetail mullet, *n*=1, coral grouper, *n*=1, and flathead gray mullet, *n*=3.	Kim et al. (2011 [PMID:21531423])
ditBu-BZT	3846-71-7	Fish, muscle tissue of 3 spp.	Manila Bay, Philippines	Range of means/single values 0.78-9.60 ng/g lipid wt.	The species were bluetail mullet, *n*=1, coral grouper, *n*=1, and flathead gray mullet, *n*=3.	Kim et al. (2011 [PMID:21531423])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
ditBu-ClBZT	3864-99-1	Fish, muscle tissue of 3 spp.	Manila Bay, Philippines	Range of means/single values 2.57-18.5 ng/g lipid wt.	The species were bluetail mullet, *n*=1, coral grouper, *n*=1, and flathead gray mullet, *n*=3.	Kim et al. (2011 [PMID:21531423])
Bumetrizole	3896-11-5	Fish, muscle tissue of 3 spp.	Manila Bay, Philippines	Range of means/single values <MDL to 211 ng/g lipid wt.	The species were bluetail mullet, *n*=1, coral grouper, *n*=1, and flathead gray mullet, *n*=3. [MDL = method detection limit.]	Kim et al. (2011 [PMID:21531423])
diMeEtPh-BZT	70321-86-7	Fish, muscle tissue of 3 spp.	Manila Bay, Philippines	Range of means/single values ND-34.6 ng/g lipid wt.	The species were bluetail mullet, *n*=1, coral grouper, *n*=1, and flathead gray mullet, *n*=3.	Kim et al. (2011 [PMID:21531423])
ditBu-BZT	3846-71-7	Flue gas at final exit (after bag filter)	Japan, pilot-scale incinerator	0.0020 $\mu g/m^3$	Amount: 0.264 µg.	Watanabe and Noma (2010 [PMID:20227827])
ditBu-ClBZT	3864-99-1	Flue gas at final exit (after bag filter)	Japan, pilot-scale incinerator using MSW RFD	0.0042 $\mu g/m^3$	Amount: 0.554 µg Overall destruction efficiency in the incinerator >99.9999%.	Watanabe and Noma (2010 [PMID:20227827])
ditBu-BZT	3846-71-7	Fly ash	Japan, pilot-scale incinerator	0.36 µg/kg	Amount: 0.118 µg	Watanabe and Noma (2010 [PMID:20227827])
ditBu-ClBZT	3864-99-1	Fly ash	Japan, pilot-scale incinerator	0.049 µg/kg	Amount: 0.0160 µg. Ash values were somewhat lower when MSW RFD was spiked with ditBu-ClBZT at 5 g/kg.	Watanabe and Noma (2010 [PMID:20227827])
Octrizole	3147-75-9	Groundwater and sewage effluent	Bolivar, South Australia, sewage treatment plant	<LOQ	Values below the levels of quantitation (4.8 and 16 ng/L for groundwater and effluent, respectively)	Liu et al. (2011 [PMID:21704319])
Bumetrizole	3896-11-5	Groundwater and sewage effluent	Bolivar, South Australia, sewage treatment plant	<LOQ	Values below the levels of quantitation (3.3 and 11.0 ng/L in groundwater and effluent, respectively).	Liu et al. (2011 [PMID:21704319])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
Allyl-BZT	2170-39-0	Indoor dust		ND	The sources were private houses (*n*=5), a public building, car cabins (*n*=3), and SRM 2585. This was the only BZT out of 5 not detected.	Carpinteiro et al. (2010b [PMID:20435314])
Drometrizole	2440-22-4	Indoor dust		65-657 ng/g; mean = 160 ng/g, (without SRM)	The sources were private houses (*n*=5), a public building, car cabins (*n*=3), and SRM 2585.	Carpinteiro et al. (2010b [PMID:20435314])
ditPe-BZT	25973-55-1	Indoor dust		46-149 ng/g; mean = 91 ng/g (without SRM)	The sources were private houses (*n*=5), a public building, car cabins (*n*=3), and SRM 2585.	Carpinteiro et al. (2010b [PMID:20435314])
ditBu-ClBZT	3864-99-1	Indoor dust		22-127 ng/g; mean = 71 ng/g (without SRM)	The sources were private houses (*n*=5), a public building, car cabins (*n*=3), and SRM 2585.	Carpinteiro et al. (2010b [PMID:20435314])
Bumetrizole	3896-11-5	Indoor dust		42-4883 ng/g; mean = 780 ng/g (without SRM)	The sources were private houses (*n*=5), a public building, car cabins (*n*=3), and SRM 2585.	Carpinteiro et al. (2010b [PMID:20435314])
Drometrizole	2440-22-4	Indoor dust	Mainheim, Germany		Samples of dirt and exhibit scrapings vacuumed from a museum's long-term storage space were also analyzed. Drometrizole was concluded to be an artifact.	Musshoff et al. (2010 [PMID:20972535])
Drometrizole	2440-22-4	Landfill leachate		Detected	Polyinyl chloride sheets used fo seepage control in landfille [Not determined whether drometrizole was solely from sheets.]	Fukui et al. (1994)
ditBu-BZT	3846-71-7	Municipal solid waste refuse-derived fuel	Japan	7.1 µg/kg	Amount in fuel 72.8 µg. In an experiment when the compound was added at 5 g/kg, the incinerator destruction efficiency was >99.9999%.	Watanabe and Noma (2010 [PMID:20227827])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
ditBu-ClBZT	3864-99-1	Municipal solid waste refuse-derived fuel (MSW RFD)	Japan	20 μg/kg	Amount: 205 μg	Watanabe and Noma (2010 [PMID:20227827])
Drometrizole	2440-22-4	polyurethane		μg/g on plastic: 70 °C: ND 100 °C: 0.015 150 °C: 1.0 200 °C: 110 300 °C: 290	The plastics tested in the study were nitrogen-containing and non-nitrogen ones: acrylonitrile-butadiene-styrene, melamine formaldehyde, urea formaldehyde, polyethylene, polypropylene, polystyrene, polyamide 6, and polyurethane. Drometrizole was also one of only two nitrogen-containing compounds identified in emissions from polystyrene and polyolefins.	Watanabe et al. (2007 [PMID:17383710])
Allyl-BZT	2170-39-0	River and marine sediments with3% carbon content		ND	Allyl-BZT was undetected in all samples. Its LOQ was 15 ng/g.	Carpinteiro et al. (2011 [PMID:21910012])
Drometrizole	2440-22-4	River and marine sediments with3% carbon content		ND-30±4 ng/g	ND applies to 4 of 6 samples. Total carbon content ranged from 2.2-8.0% in six samples.	Carpinteiro et al. (2011 [PMID:21910012])
ditPe-BZT	25973-55-1	River and marine sediments with3% carbon content		7.9±0.7 - 56±2 ng/g	Total carbon content ranged from 2.2-8.0% in six samples.	Carpinteiro et al. (2011 [PMID:21910012])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
ditBu-BZT	3846-71-7	River and marine sediments with3% carbon content		ND-5.6±0.8 ng/g	ND applies to 5 of 6 samples. Total carbon content ranged from 2.2-8.0% in six samples.	Carpinteiro et al. (2011 [PMID:21910012])
ditBu-ClBZT	3864-99-1	River and marine sediments with3% carbon content		ND-15±2 ng/g	ND applies to 3 of 6 samples. Total carbon content ranged from 2.2-8.0% in six samples.	Carpinteiro et al. (2011 [PMID:21910012])
Bumetrizole	3896-11-5	River and marine sediments with3% carbon content		ND-32±4 ng/g	ND applies to 3 of 6 samples. Total carbon content ranged from 2.2-8.0% in six samples.	Carpinteiro et al. (2011 [PMID:21910012])
ditPe-BZT	25973-55-1	River sediments (6 sites)	China, northeastern	3.81 ng/g (2.06-7.12 ng/g) (Frequency 6/6)	Surface sediments collected in 2009 from the Songhua River downstream of 5 large cities	Zhang et al. (2011 [PMID:21480589])
ditPe-BZT	25973-55-1	River sediments (6 sites)	Saginaw and Detroit Rivers, Michigan	116 ng/g (0.72-224 ng/g) (Frequency 5/6)	Collected in 2002 downstream of Saginaw City, mouth of the Saginaw River, and Shelter Island. Detroit River collections in 1998.	Zhang et al. (2011 [PMID:21480589])
tBu-BZT	3147-76-0	River sediments (6 sites)	China, northeastern	ND	Surface sediments collected in 2009 from the Songhua River downstream of 5 large cities	Zhang et al. (2011 [PMID:21480589])
tBu-BZT	3147-76-0	River sediments (6 sites)	Saginaw and Detroit Rivers, Michigan	ND	Collected in 2002 downstream of Saginaw City, mouth of the Saginaw River, and Shelter Island. Detroit River collections in 1998.	Zhang et al. (2011 [PMID:21480589])
ditBu-ClBZT	3864-99-1	River sediments (6 sites)	China, northeastern	0.310 ng/g (Frequency 1/6)	Surface sediments collected in 2009 from the Songhua River downstream of 5 large cities	Zhang et al. (2011 [PMID:21480589])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
ditBu-ClBZT	3864-99-1	River sediments (6 sites)	Saginaw and Detroit Rivers, Michigan	0.850 ng/g (0.22-1.90 ng/g) (Frequency 3/6)	Collected in 2002 downstream of Saginaw City, mouth of the Saginaw River, and Shelter Island. Detroit River collections in 1998.	Zhang et al. (2011 [PMID:21480589])
Bumetrizole	3896-11-5	River sediments (6 sites)	China, northeastern	1.86 ng/g (1.71-2.01 ng/g) (Frequency 6/6)	Surface sediments collected in 2009 from the Songhua River downstream of 5 large cities	Zhang et al. (2011 [PMID:21480589])
Bumetrizole	3896-11-5	River sediments (6 sites)	Saginaw and Detroit Rivers, Michigan	5.88 ng/g (1/6)	Collected in 2002 downstream of Saginaw City, mouth of the Saginaw River, and Shelter Island. Detroit River collections in 1998.	Zhang et al. (2011 [PMID:21480589])
Drometrizole	2440-22-4	Rivers and lakes, background sites (5) [Sediments]	Japan (Saitama Prefecture north of Tokyo; population ~1 million)	ND [1.3 µg/kg dry wt.]	When given in this publication, mean values are geometric means calculated from detected samples. [Sediment frequency 1/5]. Sampling in summer 2008.	Kameda et al. (2011 [PMID:21429641])
ditPe-BZT	25973-55-1	Rivers and lakes, background sites (5) [Sediments]	Japan	ND [58 (29-89) µg/kg dry wt.]	[Sediment frequency 3/5]	Kameda et al. (2011 [PMID:21429641])
Octrizole	3147-75-9	Rivers and lakes, background sites (5) [Sediments]	Japan	ND [ND]		Kameda et al. (2011 [PMID:21429641])
ditBu-ClBZT	3864-99-1	Rivers and lakes, background sites (5) [Sediments]	Japan	ND [0.7 (0.5-1.1) µg/kg dry wt.]	[Sediment frequency 2/5]	Kameda et al. (2011 [PMID:21429641])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
Bumetrizole	3896-11-5	Rivers and lakes, background sites (5) [Sediments]	Japan	ND [1.2 (1.1-1.3) µg/kg dry wt.]	[Sediment frequency 2/5]	Kameda et al. (2011 [PMID:21429641])
diMeEtPh-BZT	70321-86-7	Rivers and lakes, background sites (5) [Sediments]	Japan	ND [39 (8.3-113) µg/kg dry wt.]	[Sediment frequency 3/5]	Kameda et al. (2011 [PMID:21429641])
Drometrizole	2440-22-4	Rivers, heavily polluted (6) [Sediments]	Japan	ND [3.4 (2.6-4.4) µg/kg dry wt.]	Frequencies 1/12 [2/6]	Kameda et al. (2011 [PMID:21429641])
ditPe-BZT	25973-55-1	Rivers, heavily polluted (6) [Sediments]	Japan	701 (149-4780) [117 (21-1735) µg/kg dry wt.]	Frequencies 4/6 [6/6]	Kameda et al. (2011 [PMID:21429641])
Octrizole	3147-75-9	Rivers, heavily polluted (6) [Sediments]	Japan	ND [26 (7.4-269) µg/kg dry wt.]	[Sediment frequency 3/6]	Kameda et al. (2011 [PMID:21429641])
ditBu-ClBZT	3864-99-1	Rivers, heavily polluted (6) [Sediments]	Japan	1 ng/L [2.4 (0.7-18) µg/kg dry wt.]	Frequencies 1/6 [5/6]	Kameda et al. (2011 [PMID:21429641])
Bumetrizole	3896-11-5	Rivers, heavily polluted (6) [Sediments]	Japan	9 ng/L [4.7 (0.9-45) µg/kg dry wt.]	Frequencies of 1/6 [5/6]	Kameda et al. (2011 [PMID:21429641])
diMeEtPh-BZT	70321-86-7	Rivers, heavily polluted (6) [Sediments]	Japan	ND [99 (38-324) µg/kg dry wt.]	[Sediment frequency 4/6]	Kameda et al. (2011 [PMID:21429641])
Drometrizole	2440-22-4	Rivers, moderately polluted (12) [Sediments]	Japan	2 ng/L [1.3 (0.5-3.3 µg/kg dry wt.)]	Frequencies 1/12 [2/12]	Kameda et al. (2011 [PMID:21429641])
ditPe-BZT	25973-55-1	Rivers, moderately polluted (12) [Sediments]	Japan	152 (30-583) ng/L [59 (10-213) µg/kg dry wt.]	Frequencies 8/12 [9/12]	Kameda et al. (2011 [PMID:21429641])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
Octrizole	3147-75-9	Rivers, moderately polluted (12) [Sediments]	Japan	ND [0.6 (0.1-4.3) µg/kg dry wt.]	[Sediment frequency 3/12]	Kameda et al. (2011 [PMID:21429641])
ditBu-ClBZT	3864-99-1	Rivers, moderately polluted (12) [Sediments]	Japan	1 (1-6) ng/L [0.0 (0.4-2.6) µg/kg dry wt.]	Frequencies 6/12 [10/12]	Kameda et al. (2011 [PMID:21429641])
Bumetrizole	3896-11-5	Rivers, moderately polluted (12) [Sediments]	Japan	2 (1-22) ng/L [1.8 (1.0-5.0) µg/kg dry wt.]	Frequencies of 5/12 [12/12]	Kameda et al. (2011 [PMID:21429641])
diMeEtPh-BZT	70321-86-7	Rivers, moderately polluted (12) [sediments]	Japan	ND [47 (18-315) µg/kg dry wt.]	[Sediment frequency 8/12]	Kameda et al. (2011 [PMID:21429641])
Drometrizole	2440-22-4	Sediments	Near a small specialty chemicals plant	2-670 ppm		Hites et al. (1979); Jungclaus et al. (1978)
ditPe-BZT	25973-55-1	Sediments	Near a small specialty chemicals plant	1-100 ppm		Hites et al. (1979); Jungclaus et al. (1978)
tBu-BZT	3147-76-0	Sediments	Near a small specialty chemicals plant	60 ppm		Hites et al. (1979); Jungclaus et al. (1978)
tBu-ClBZT	3287-17-0	Sediments	Near a small specialty chemicals plant	2-50 ppm		Hites et al. (1979); Jungclaus et al. (1978)
ditBu-BZT	3846-71-7	Sediments	Near a small specialty chemicals plant	40 ppm		Hites et al. (1979); Jungclaus et al. (1978)
ditBu-ClBZT	3864-99-1	Sediments	Near a small specialty chemicals plant	2-300 ppm		Hites et al. (1979); Jungclaus et al. (1978)
ditPe-BZT	25973-55-1	Sediments from the Ariake Sea	Japan – Chikugo River, mouths 1 and 1	5.0 and 6.3 ng/g dry wt., respectively		Nakata et al. (2009 [PMID:19806721])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
ditPe-BZT	25973-55-1	Sediments from the Ariake Sea	Japan – Yabe River mouth	4.5 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditPe-BZT	25973-55-1	Sediments from the Ariake Sea	Japan – Omuta River mouth	16 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditPe-BZT	25973-55-1	Sediments from the Ariake Sea	Japan – Kikuchi River mouths 1 and 2	2.6 and 5.0 ng/g dry wt., respectively		Nakata et al. (2009 [PMID:19806721])
ditPe-BZT	25973-55-1	Sediments from the Ariake Sea	Japan – Tojin River mouth	8.1 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditPe-BZT	25973-55-1	Sediments from the Ariake Sea	Japan – Kumamoto Port	4.2 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditPe-BZT	25973-55-1	Sediments from the Ariake Sea	Japan – Midori River mouth	11 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditPe-BZT	25973-55-1	Sediments from the Ariake Sea	Japan – Shiranui coast	3.8 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditPe-BZT	25973-55-1	Sediments from the Ariake Sea	Japan – Hikawa River mouth	2.8 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditPe-BZT	25973-55-1	Sediments from the Ariake Sea	Japan – Omuta River (5 samples)	18-320 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-BZT	3846-71-7	Sediments from the Ariake Sea	Japan – Chikugo River, mouths 1 and 1	0.8 ng/g dry wt. (both)		Nakata et al. (2009 [PMID:19806721])
ditBu-BZT	3846-71-7	Sediments from the Ariake Sea	Japan – Yabe River mouth	0.8 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-BZT	3846-71-7	Sediments from the Ariake Sea	Japan – Omuta River mouth	2.3 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
ditBu-BZT	3846-71-7	Sediments from the Ariake Sea	Japan – Kikuchi River mouths 1 and 2	1.2 and 1.1 ng/g dry wt., respectively		Nakata et al. (2009 [PMID:19806721])
ditBu-BZT	3846-71-7	Sediments from the Ariake Sea	Japan – Tojin River mouth	1.1 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-BZT	3846-71-7	Sediments from the Ariake Sea	Japan – Kumamoto Port	1.0 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-BZT	3846-71-7	Sediments from the Ariake Sea	Japan – Midori River mouth	0.3 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-BZT	3846-71-7	Sediments from the Ariake Sea	Japan – Shiranui coast	0.3 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-BZT	3846-71-7	Sediments from the Ariake Sea	Japan – Hikawa River mouth	0.3 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-BZT	3846-71-7	Sediments from the Ariake Sea	Japan – Omuta River (5 samples)	2.6-14 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-ClBZT	3864-99-1	Sediments from the Ariake Sea	Japan – Chikugo River, mouths 1 and 1	1.8 and 1.9 ng/g dry wt., respectively		Nakata et al. (2009 [PMID:19806721])
ditBu-ClBZT	3864-99-1	Sediments from the Ariake Sea	Japan – Yabe River mouth	1.6 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-ClBZT	3864-99-1	Sediments from the Ariake Sea	Japan – Omuta River mouth	9.9 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-ClBZT	3864-99-1	Sediments from the Ariake Sea	Japan – Kikuchi River mouths 1 and 2	1.6 and 2.4 ng/g dry wt., respectively		Nakata et al. (2009 [PMID:19806721])
ditBu-ClBZT	3864-99-1	Sediments from the Ariake Sea	Japan – Tojin River mouth	3.2 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
ditBu-ClBZT	3864-99-1	Sediments from the Ariake Sea	Japan – Kumamoto Port	2.0 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-ClBZT	3864-99-1	Sediments from the Ariake Sea	Japan – Midori River mouth	3.2 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-ClBZT	3864-99-1	Sediments from the Ariake Sea	Japan – Shiranui coast	6.3 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-ClBZT	3864-99-1	Sediments from the Ariake Sea	Japan – Hikawa River mouth	1.6 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
ditBu-ClBZT	3864-99-1	Sediments from the Ariake Sea	Japan – Omuta River (5 samples)	16-190 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
Bumetrizole	3896-11-5	Sediments from the Ariake Sea	Japan – Chikugo River, mouths 1 and 1	1.8 and 2.0 ng/g dry wt., respectively		Nakata et al. (2009 [PMID:19806721])
Bumetrizole	3896-11-5	Sediments from the Ariake Sea	Japan – Yabe River mouth	1.5 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
Bumetrizole	3896-11-5	Sediments from the Ariake Sea	Japan – Omuta River mouth	12 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
Bumetrizole	3896-11-5	Sediments from the Ariake Sea	Japan – Kikuchi River mouths 1 and 2	2.7 and 3.3 ng/g dry wt., respectively		Nakata et al. (2009 [PMID:19806721])
Bumetrizole	3896-11-5	Sediments from the Ariake Sea	Japan – Tojin River mouth	2.6 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
Bumetrizole	3896-11-5	Sediments from the Ariake Sea	Japan – Kumamoto Port	1.8 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
Bumetrizole	3896-11-5	Sediments from the Ariake Sea	Japan – Midori River mouth	5.4 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
Bumetrizole	3896-11-5	Sediments from the Ariake Sea	Japan – Shiranui coast	4.8 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
Bumetrizole	3896-11-5	Sediments from the Ariake Sea	Japan – Hikawa River mouth	3.2 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
Bumetrizole	3896-11-5	Sediments from the Ariake Sea	Japan – Omuta River (5 samples)	23-200 ng/g dry wt.		Nakata et al. (2009 [PMID:19806721])
Allyl-BZT	2170-39-0	Sewage (raw)	Urban sewage treatment plant in Spain	ND		Carpinteiro et al. (2010a [PMID:20229350])
Drometrizole	2440-22-4	Sewage (raw)	Urban sewage treatment plant in Spain	ND-16±1 ng/L (ppt)		Carpinteiro et al. (2010a [PMID:20229350])
ditPe-BZT	25973-55-1	Sewage (raw)	Urban sewage treatment plant in Spain	ND-19±2 ng/L (ppb)		Carpinteiro et al. (2010a [PMID:20229350])
ditBu-ClBZT	3864-99-1	Sewage (raw)	Urban sewage treatment plant in Spain	ND		Carpinteiro et al. (2010a [PMID:20229350])
Bumetrizole	3896-11-5	Sewage (raw)	Urban sewage treatment plant in Spain (5 samples)	ND-57±9 ng/L (ppt)		Carpinteiro et al. (2010a [PMID:20229350])
Octrizole	3147-75-9	Sewage biosolid	Bolivar, South Australia, sewage treatment plant	122.9±7.1 ng/g	Bolivar is an outer northern suburb of Adelaide.	Liu et al. (2011 [PMID:21704319])
Bumetrizole	3896-11-5	Sewage biosolid	Bolivar, South Australia, sewage treatment plant	49.9±7.4 ng/g		Liu et al. (2011 [PMID:21704319])
ditBu-ClBZT	3864-99-1	Sewage effluent	Japan, 5 WWTPs	All values <8.7 ng/L	No mean calculable	Nakata and Shinohara (2010)
ditPe-BZT	25973-55-1	Sewage influent	Japan, 5 WWTPs	34±15 ng/L (18-52 ng/L)		Nakata and Shinohara (2010)

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
ditBu-ClBZT	3864-99-1	Sewage influent	Japan, 5 wastewater (sewage) treatment plants (WWTPs)	(<8.7-12 ng/L)	No mean calculable; three values <8.7 ng/L.	Nakata and Shinohara (2010)
Bumetrizole	3896-11-5	Sewage influent	Japan, 5 WWTPs	46±22 ng/L (24-78 ng/L)		Nakata and Shinohara (2010)
ditPe-BZT	25973-55-1	Sewage plant treated effluent	Japan, 5 WWTPs	2.6±0.32 ng/L (2.1-2.9 ng/L)		Nakata and Shinohara (2010)
Bumetrizole	3896-11-5	Sewage plant treated effluent	Japan, 5 WWTPs	3.6±0.65 ng/L (3.0-4.5 ng/L)		Nakata and Shinohara (2010)
ditBu-ClBZT	3864-99-1	Sewage sludge	Japan, 5 WWTPs	170±33 ng/g dry wt. (120-200 ng/g)		Nakata and Shinohara (2010)
ditBu-ClBZT	3864-99-1	Sewage sludge (5)	China, northeastern	3.68 ng/g (1.80-8.40 ng/g) (5/5)	Collected in July 2009 from 5 WWTPs serving 5 large cities along the Songhua River	Zhang et al. (2011 [PMID:21480589])
ditPe-BZT	25973-55-1	Sewage sludge (mean 31±2.2% carbon)	Japan, 5 WWTPs	510 ±67 ng/g dry wt. (430-570 ng/g)		Nakata and Shinohara (2010)
Bumetrizole	3896-11-5	Sewage sludge (mean 31±2.2% carbon)	Japan, 5 WWTPs	1,100±460 ng/g dry wt. (760-1800 ng/g)		Nakata and Shinohara (2010)
ditPe-BZT	25973-55-1	Sewage sludges (5)	China, northeastern	1300 ng/g (40.6-5920 ng/g) (4/5)	Collected in July 2009 from 5 WWTPs serving 5 large cities along the Songhua River	Zhang et al. (2011 [PMID:21480589])
tBu-BZT	3147-76-0	Sewage sludges (5)	China, northeastern WWTPs	0.955 ng/g dry wt. (0.730-1.18 ng/g)	Collected in July 2009 from 5 WWTPs serving 5 large cities along the Songhua River. Frequency: 2/5	Zhang et al. (2011 [PMID:21480589])
Bumetrizole	3896-11-5	Sewage sludges (5)	China, northeastern	77.4 ng/g (23.3-136 ng/g) (5/5)	Collected in July 2009 from 5 WWTPs serving 5 large cities along the Songhua River	Zhang et al. (2011 [PMID:21480589])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
Drometrizole	2440-22-4	Sewage treatment plant effluents (4) [Sediments]	Japan	7 (3-23) ng/L [ND]	Frequencies ¾ [0/4]	Kameda et al. (2011 [PMID:21429641])
ditPe-BZT	25973-55-1	Sewage treatment plant effluents (4) [Sediments]	Japan	62 (47-88) ng/L [13 (10-85) µg/kg dry wt.]	Frequencies 3/4 [4/4]	Kameda et al. (2011 [PMID:21429641])
Octrizole	3147-75-9	Sewage treatment plant effluents (4) [Sediments]	Japan	ND [ND]		Kameda et al. (2011 [PMID:21429641])
ditBu-ClBZT	3864-99-1	Sewage treatment plant effluents (4) [Sediments]	Japan	2 ng/L [0.5 (0.3-1.0) µg/kg dry wt.]	Frequencies 1 of 4 [4/4]	Kameda et al. (2011 [PMID:21429641])
Bumetrizole	3896-11-5	Sewage treatment plant effluents (4) [Sediments]	Japan	13 ng/L [0.8 (0.4-5.4) µg/kg dry wt.]	Frequencies of 1 of 4 [4/4]	Kameda et al. (2011 [PMID:21429641])
diMeEtPh-BZT	70321-86-7	Sewage treatment plant effluents (4) [Sediments]	Japan	ND [ND]		Kameda et al. (2011 [PMID:21429641])
Drometrizole	2440-22-4	Streams (2) [Sediments]	Japan	10 ng/L [15 µg/kg dry wt.]	Frequencies ½ [1/2]	Kameda et al. (2011 [PMID:21429641])
ditPe-BZT	25973-55-1	Streams (2) [Sediments]	Japan	70 ng/L [102 (10-1146) µg/kg dry wt.]	Frequencies 1 of 2 [2/2]	Kameda et al. (2011 [PMID:21429641])
Octrizole	3147-75-9	Streams (2) [Sediments]	Japan	ND [1266 µg/kg dry wt.]	[Sediment frequency 1 of 2]	Kameda et al. (2011 [PMID:21429641])
ditBu-ClBZT	3864-99-1	Streams (2) [Sediments]	Japan	5 ng/L [4.7 (0.6-3.7) µg/kg dry wt.]	Frequencies 1 of 2 [2/2]	Kameda et al. (2011 [PMID:21429641])
Bumetrizole	3896-11-5	Streams (2) [Sediments]	Japan	16 ng/L [7.8 (0.6-110 µg/kg dry wt.]	Frequencies 1 of 2 [2/2]	Kameda et al. (2011 [PMID:21429641])
diMeEtPh-BZT	70321-86-7	Streams (2) [Sediments]	Japan	ND [1266µg/kg dry wt.]	[Sediment frequency 1/2]	Kameda et al. (2011 [PMID:21429641])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
Drometrizole	2440-22-4	Water	Near a small specialty chemicals plant	0.5-7 ppm in wastewater and 0.006-0.10 ppm in river water		Hites et al. (1979); Jungclaus et al. (1978)
ditPe-BZT	25973-55-1	Water	Near a small specialty chemicals plant	0.55-4.7 ppm in wastewater and 0.007-0.085 ppm in river water		Hites et al. (1979); Jungclaus et al. (1978)
tBu-BZT	3147-76-0	Water	Near a small specialty chemicals plant	ND		Hites et al. (1979); Jungclaus et al. (1978)
tBu-ClBZT	3287-17-0	Water	Near a small specialty chemicals plant	ND		Hites et al. (1979); Jungclaus et al. (1978)
ditBu-BZT	3846-71-7	Water	Near a small specialty chemicals plant	ND		Hites et al. (1979); Jungclaus et al. (1978)
ditBu-ClBZT	3864-99-1	Water	Near a small specialty chemicals plant	ND		Hites et al. (1979); Jungclaus et al. (1978)
Drometrizole	2440-22-4	Water and sediment samples from paper-recycling process water discharge areas	Shizuoka Prefecture, Japan	Water (µg/L) site 1: 13 site 2: ND site 3: 0.22 site 4: ND site 5: ND Sediment (µg/g) Site 1: 8.4 Site 3: 0.31	Outfall watershed sites: Site 1 = adjacent area Site 2 = upstream Site 3 = downstream No sediment samples were taken from Sites 2, 4, and 5.	Terasaki et al. (2007 [PMID:17941731])

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
Drometrizole	2440-22-4	Water and sediments – Narragansett Bay sediment core	Narragansett Bay (in 1997)	Max: 10.5 µg/g (4-6 cm core) Bound: 614 ng/g at surface; 26.2 ng/g at 8-10 cm, and ND at 10-13 cm	This was the only benzotriazole detected in the bound fraction of the core. Bumetrizole, tBu-BZT, and tBu-ClBZT were also detected; their results were not reported since they were substantially less than this finding.	Reddy et al. (2000)
ditPe-BZT	25973-55-1	Water and sediments – Narragansett Bay sediment core	Narragansett Bay (in 1997)	Max: ~25 µg/g	Bumetrizole, tBu-BZT, and tBu-ClBZT were also detected; their results were not reported since they were substantially less than this finding.	Reddy et al. (2000)
ditBu-ClBZT	3864-99-1	Water and sediments – Narragansett Bay sediment core	Narragansett Bay (in 1997)	Max: ~25 µg/g	Bumetrizole, tBu-BZT, and tBu-ClBZT were also detected; their results were not reported since they were substantially less than this finding.	Reddy et al. (2000)
Drometrizole	2440-22-4	Water and sediments – Pawtuxet River core	Pawtuxet River (in 1989)	In 10-12 cm: Free: 4300 µg/g Bound: 29 µg/g	One of two most abundant benzotriazoles detected. It was found down to the 50-52 cm Free refers to fraction that was removed with organic solvent extractions.	Reddy et al. (2000)
ditPe-BZT	25973-55-1	Water and sediments – Pawtuxet River core	Pawtuxet River (in 1989)	In 10-12 cm: Free: Trace levels Bound: ND	This was found only in the top 20 cm of the core. Free refers to fraction that was removed with organic solvent extractions.	Reddy et al. (2000)
tBu-BZT	3147-76-0	Water and sediments – Pawtuxet River core	Pawtuxet River (in 1989)	In 10-12 cm: Free: 130 µg/g Bound: 260 ng/g	This was found only in the top 20 cm of the core. Free refers to fraction that was removed with organic solvent extractions.	Reddy et al. (2000)
tBu-ClBZT	3287-17-0	Water and sediments – Pawtuxet River core	Pawtuxet River (in 1989)	In 10-12 cm: Free: 71 µg/g Bound: 740 ng/g	This was found only in the top 20 cm of the core. Free refers to fraction that was removed with organic solvent extractions.	Reddy et al. (2000)

Compound	CASRN	Medium	Location	Concentration	Comment	Reference
ditBu-ClBZT	3864-99-1	Water and sediments – Pawtuxet River core	Pawtuxet River (in 1989)	In 10-12 cm: Free: 5200 µg/g Bound: 1000 ng/g	One of two most abundant benzotriazoles detected. It was found down to the 50-52 cm core. Free refers to fraction that was removed with organic solvent extractions.	Reddy et al. (2000)
Bumetrizole	3896-11-5	Water and sediments – Pawtuxet River core	Pawtuxet River (in 1989)	In 10-12 cm: Free: 260 µg/g Bound: 110 ng/g	This was found only in the top 20 cm of the core. Free refers to fraction that was removed with organic solvent extractions.	Reddy et al. (2000)

Abbreviations: CASRN = Chemical Abstracts Registry Number, LOQ = limit of quantification, MSW RFD = municipal solid waste refuse-derived fuel, ND = not detected, ppb = parts-per-billion, ppm = parts-per-million, ppt = parts-per-trillion, spp. = species, wt. = weight

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Appendix E. Leadscope Results

CAS Number	Genetic Toxicity													
	mouse lymphoma		hgprt		mam. mutation DL		mam. mutation		drosophila SLRL		drosophila HT		drosophila	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	ND		Neg.	0.239	Neg.	0.0346	Neg.	0.0584	Neg.	0.288	Neg.	0.0392	Neg.	0.168
2440-22-4	Neg.	0.438	Neg.	0.229	Neg.	0.0344	Neg.	0.0479	Neg.	0.213	ND		Neg.	0.0874
3147-76-0	Neg.	0.4005	Neg.	0.1935	Neg.	0.0388	Neg.	0.0601	Neg.	0.139	ND		Neg.	0.059
3287-17-0	Neg.	0.3945	Neg.	0.168	Neg.	0.00425	Neg.	0.0163	Neg.	0.069	ND		Neg.	0.0363
3147-75-9	Neg.	0.2985	Neg.	0.1302	Neg.	0.0553	Neg.	0.0734	Neg.	0.0885	Neg.	0.00402	Neg.	0.0482
96549-95-0	Neg.	0.416	Neg.	0.214	Neg.	0.0451	Neg.	0.0679	Neg.	0.334	ND		Neg.	0.116
83741-30-4	Neg.	0.326	Neg.	0.148	ND		ND		Neg.	0.164	ND		Neg.	0.098
96478-09-0	**Pos.**	0.968	ND		ND		ND		ND		ND		ND	
23328-53-2	Neg.	0.0829	Neg.	0.0478	Neg.	0.086	Neg.	0.0743	Neg.	0.0604	ND		Neg.	0.0406
36437-37-3	Neg.	0.302	Neg.	0.0989	Neg.	0.055	Neg.	0.0731	Neg.	0.0855	ND		Neg.	0.0387
3896-11-5	Neg.	0.2945	Neg.	0.1186	Neg.	0.00422	Neg.	0.0132	Neg.	0.0663	ND		Neg.	0.0287
3846-71-7	Neg.	0.3845	Neg.	0.1278	Neg.	0.0398	Neg.	0.0597	Neg.	0.13	ND		Neg.	0.0445
3864-99-1	Neg.	0.363	Neg.	0.1251	Neg.	0.00463	Neg.	0.0166	Neg.	0.0584	ND		Neg.	0.0237
25973-55-1	Neg.	0.281	Neg.	0.08505	Neg.	0.0607	Neg.	0.0763	Neg.	0.0767	ND		Neg.	0.0328
70693-49-1	Neg.	0.255	Neg.	0.0766	Neg.	0.0646	Neg.	0.0763	Neg.	0.0715	ND		Neg.	0.0294
73936-91-1	Neg.	0.2025	Neg.	0.05535	Neg.	0.0361	Neg.	0.0753	Neg.	0.0264	ND		Neg.	0.0231
207738-63-4	Neg.	0.183	Neg.	0.05815	Neg.	0.0399	Neg.	0.0778	Neg.	0.0144	ND		Neg.	0.0152
70321-86-7	Neg.	0.2775	Neg.	0.09835	Neg.	0.0263	Neg.	0.062	Neg.	0.0421	ND		Neg.	0.0267
84268-36-0	Neg.	0.1645	Neg.	0.0374	Neg.	0.0679	Neg.	0.0841	Neg.	0.0656	ND		Neg.	0.0346
84268-33-7	Neg.	0.207	Neg.	0.0594	Neg.	0.0696	Neg.	0.0964	Neg.	0.0118	ND		Neg.	0.0155
84268-08-6	Neg.	0.117	Neg.	0.0402	Neg.	0.141	Neg.	0.119	Neg.	0.0214	ND		Neg.	0.023
84268-23-5	Neg.	0.0714	Neg.	0.02985	Neg.	0.146	Neg.	0.123	Neg.	0.0146	ND		Neg.	0.0222
83044-89-7	Neg.	0.0698	Neg.	0.0159	Neg.	0.0178	Neg.	0.035	Neg.	0.00674	ND		Neg.	0.0134
103597-45-1	Neg.	0.204	Neg.	0.0568	Neg.	0.0862	Neg.	0.0875	Neg.	0.0605	ND		Neg.	0.0203
27876-55-7	Neg.	0.275	Neg.	0.143	Neg.	0.057	Neg.	0.0732	Neg.	0.0778	ND		Neg.	0.0394
3147-77-1	Neg.	0.1423	Neg.	0.1148	Neg.	0.0607	Neg.	0.0374	Neg.	0.113	Neg.	0.0202	Neg.	0.0843
2170-39-0	Neg.	0.364	Neg.	0.1282	Neg.	0.0415	Neg.	0.0517	Neg.	0.102	ND		Neg.	0.0473

CAS Number	Genetic Toxicity													
	E. coli		salmonella		microbial		E. coli w		yeast		s. cerevisiae		UDS	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	Neg.	0.465	**Pos.**	0.514	**Pos.**	0.553	Neg.	0.162	Neg.	0.4585	Neg.	0.3705	Neg.	0.294
2440-22-4	Neg.	0.38	**Pos.**	0.504	Neg.	0.366	Neg.	0.0705	Neg.	0.3725	Neg.	0.3195	Neg.	0.393
3147-76-0	Neg.	0.118	Neg.	0.217	Neg.	0.0983	Neg.	0.0102	Neg.	0.157	Neg.	0.1125	Neg.	0.212
3287-17-0	Neg.	0.0822	Neg.	0.109	Neg.	0.0407	Neg.	0.00536	Neg.	0.1376	Neg.	0.06155	Neg.	0.154
3147-75-9	Neg.	0.0768	Neg.	0.0665	Neg.	0.0335	Neg.	0.00475	Neg.	0.1088	Neg.	0.07435	Neg.	0.0688
96549-95-0	Neg.	0.457	Neg.	0.347	Neg.	0.264	Neg.	0.0384	Neg.	0.287	ND		Neg.	0.301
83741-30-4	Neg.	0.0138	Neg.	0.42	**Pos.**	0.53	Neg.	0.016	Neg.	0.336	ND		Neg.	0.383
96478-09-0	Neg.	0.0111	Neg.	0.256	Neg.	0.153	Neg.	0.00167	ND		ND		Neg.	0.205
23328-53-2	Neg.	0.0174	Neg.	0.0255	Neg.	0.0514	Neg.	0.00116	Neg.	0.06228	Neg.	0.008085	Neg.	0.122
36437-37-3	Neg.	0.0847	Neg.	0.114	Neg.	0.0662	Neg.	0.00565	Neg.	0.1298	Neg.	0.0779	Neg.	0.0634
3896-11-5	Neg.	0.0771	Neg.	0.108	Neg.	0.0413	Neg.	0.0151	Neg.	0.1343	Neg.	0.05755	Neg.	0.149
3846-71-7	Neg.	0.108	Neg.	0.21	Neg.	0.107	Neg.	0.00777	Neg.	0.1316	Neg.	0.08395	Neg.	0.136
3864-99-1	Neg.	0.072	Neg.	0.0952	Neg.	0.0374	Neg.	0.00426	Neg.	0.0961	Neg.	0.03975	Neg.	0.104
25973-55-1	Neg.	0.0796	Neg.	0.089	Neg.	0.0574	Neg.	0.00549	Neg.	0.1004	Neg.	0.05995	Neg.	0.0522
70693-49-1	Neg.	0.0637	Neg.	0.0545	Neg.	0.0344	Neg.	0.00319	Neg.	0.06025	Neg.	0.035	Neg.	0.0414
73936-91-1	Neg.	0.0158	Neg.	0.0396	Neg.	0.0428	Neg.	0.00197	Neg.	0.003465	ND		Neg.	0.0209
207738-63-4	Neg.	0.0133	Neg.	0.0343	Neg.	0.04	Neg.	0.00182	ND		ND		Neg.	0.0914
70321-86-7	Neg.	0.00887	Neg.	0.133	Neg.	0.134	Neg.	0.00261	Neg.	0.00441	ND		Neg.	0.0686
84268-36-0	Neg.	0.0621	Neg.	0.0408	Neg.	0.0196	Neg.	0.0103	ND		ND		Neg.	0.0345
84268-33-7	Neg.	0.0295	Neg.	0.109	Neg.	0.0565	Neg.	0.00518	ND		ND		Neg.	0.0558
84268-08-6	Neg.	0.00575	Neg.	0.063	Neg.	0.0355	Neg.	0.00321	ND		ND		Neg.	0.0406
84268-23-5	Neg.	0.00365	Neg.	0.0336	Neg.	0.0314	Neg.	0.00109	ND		ND		Neg.	0.0283
83044-89-7	ND		Neg.	0.0151	Neg.	0.0124	ND		ND		ND		ND	
103597-45-1	Neg.	0.0653	Neg.	0.0392	Neg.	0.107	Neg.	0.00282	Neg.	0.0109	ND		Neg.	0.0203
27876-55-7	Neg.	0.0731	Neg.	0.0828	Neg.	0.0423	Neg.	0.00445	Neg.	0.03865	Neg.	0.03665	Neg.	0.0722
3147-77-1	Neg.	0.195	Neg.	0.143	Neg.	0.0786	Neg.	0.0325	Neg.	0.2169	Neg.	0.03185	Neg.	0.103
2170-39-0	Neg.	0.282	Neg.	0.366	Neg.	0.28	Neg.	0.0319	Neg.	0.276	ND		Neg.	0.438

CAS Number	Genetic Toxicity													
	UDS human lymphocytes		UDS rat hepatocytes		In vitro composite		In vitro chrom. ab. other cells		In vitro chrom. ab. HL cells		In vitro chrom. ab. CHO		In vitro chrom. ab. CHL	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	Neg.	0.319	Neg.	0.229	Neg.	0.401	Neg.	0.437	**Pos.**	0.607	Neg.	0.305	Neg.	0.4155
2440-22-4	Neg.	0.374	Neg.	0.243	Neg.	0.3315	Neg.	0.179	ND		Neg.	0.202	Neg.	0.412
3147-76-0	Neg.	0.247	Neg.	0.139	Neg.	0.15	Neg.	0.0991	ND		Neg.	0.0916	Neg.	0.2545
3287-17-0	Neg.	0.242	Neg.	0.135	Neg.	0.1435	Neg.	0.0917	ND		Neg.	0.08685	Neg.	0.265
3147-75-9	Neg.	0.185	Neg.	0.0557	Neg.	0.07795	Neg.	0.0805	Neg.	0.0605	Neg.	0.06985	Neg.	0.138
96549-95-0	Neg.	0.307	ND		Neg.	0.249	ND		ND		ND		Neg.	0.305
83741-30-4	Neg.	0.346	ND		Neg.	0.3665	ND		Neg.	0.221	**Pos.**	0.5035	Neg.	0.3185
96478-09-0	Neg.	0.206	ND		**Pos.**	0.5325	ND		ND		Neg.	0.345	**Pos.**	0.5285
23328-53-2	Neg.	0.131	Neg.	0.0391	Neg.	0.0357	Neg.	0.0127	Neg.	0.0472	Neg.	0.00523	Neg.	0.0501
36437-37-3	Neg.	0.12	Neg.	0.0967	Neg.	0.09055	Neg.	0.0665	ND		Neg.	0.02567	Neg.	0.1236
3896-11-5	Neg.	0.195	Neg.	0.164	Neg.	0.14	Neg.	0.0732	ND		Neg.	0.0441	Neg.	0.2205
3846-71-7	Neg.	0.154	Neg.	0.126	Neg.	0.133	Neg.	0.0686	ND		Neg.	0.03415	Neg.	0.1975
3864-99-1	Neg.	0.157	Neg.	0.117	Neg.	0.1095	Neg.	0.0508	ND		Neg.	0.02805	Neg.	0.1808
25973-55-1	Neg.	0.121	Neg.	0.0866	Neg.	0.06745	Neg.	0.0483	ND		Neg.	0.02063	Neg.	0.08985
70693-49-1	Neg.	0.108	Neg.	0.0411	Neg.	0.0495	Neg.	0.0357	ND		Neg.	0.01809	Neg.	0.0788
73936-91-1	Neg.	0.0213	Neg.	0.0376	Neg.	0.04815	Neg.	0.0124	Neg.	0.0221	Neg.	0.0072	Neg.	0.1885
207738-63-4	Neg.	0.052	ND		Neg.	0.0331	Neg.	0.00146	Neg.	0.0179	Neg.	0.003385	Neg.	0.1552
70321-86-7	Neg.	0.0282	ND		Neg.	0.08435	Neg.	0.0127	Neg.	0.0328	Neg.	0.00856	Neg.	0.2935
84268-36-0	Neg.	0.0167	Neg.	0.0682	Neg.	0.05755	Neg.	0.0313	ND		Neg.	0.0236	Neg.	0.09845
84268-33-7	Neg.	0.0487	ND		Neg.	0.09235	Neg.	0.112	ND		Neg.	0.02445	Neg.	0.07025
84268-08-6	Neg.	0.0276	ND		Neg.	0.0503	Neg.	0.0444	ND		Neg.	0.01366	Neg.	0.02745
84268-23-5	Neg.	0.026	ND		Neg.	0.0356	Neg.	0.0127	ND		Neg.	0.004795	Neg.	0.0196
83044-89-7	ND		ND		Neg.	0.0338	Neg.	0.0117	ND		Neg.	0.00449	Neg.	0.02045
103597-45-1	Neg.	0.0201	ND		Neg.	0.02855	Neg.	0.0116	Neg.	0.0161	Neg.	0.00525	Neg.	0.1206
27876-55-7	Neg.	0.186	Neg.	0.0627	Neg.	0.0606	Neg.	0.0407	ND		Neg.	0.05568	Neg.	0.1491
3147-77-1	Neg.	0.167	ND		Neg.	0.1724	Neg.	0.11	Neg.	0.192	Neg.	0.176	Neg.	0.2825
2170-39-0	Neg.	0.248	Neg.	0.321	Neg.	0.2345	Neg.	0.132	ND		Neg.	0.1094	Neg.	0.2485

CAS Number	Genetic Toxicity															
	SCE in vitro		SCE in vitro CHO		SCE in vitro other cells		chrom. ab.		chrom. ab. other rodent		chrom. ab. rat		micronucleus mouse		micronucleus rodent	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	**Pos.**	0.531	**Pos.**	0.755	**Pos.**	0.969	Neg.	0.0686	Neg.	0.27	Neg.	0.107	Neg.	0.452	Neg.	0.313
2440-22-4	Neg.	0.4137	**Pos.**	0.66	**Pos.**	0.541	Neg.	0.022	Neg.	0.171	Neg.	0.0691	Neg.	0.328	Neg.	0.199
3147-76-0	Neg.	0.2297	**Pos.**	0.522	Neg.	0.207	Neg.	0.00696	Neg.	0.214	Neg.	0.0605	Neg.	0.235	Neg.	0.146
3287-17-0	Neg.	0.1682	Neg.	0.383	Neg.	0.493	Neg.	0.00689	Neg.	0.105	Neg.	0.0673	Neg.	0.231	Neg.	0.142
3147-75-9	Neg.	0.161	Neg.	0.321	Neg.	0.197	Neg.	0.001	Neg.	0.128	Neg.	0.0551	Neg.	0.179	Neg.	0.108
96549-95-0	Neg.	0.331	**Pos.**	0.598	Neg.	0.48	ND		ND		ND		Neg.	0.255	Neg.	0.154
83741-30-4	Neg.	0.4395	**Pos.**	0.633	**Pos.**	0.955	Neg.	0.291	ND		Neg.	0.0335	Neg.	0.301	Neg.	0.166
96478-09-0	Neg.	0.285	**Pos.**	0.88	ND		ND		ND		ND		ND		Neg.	0.144
23328-53-2	Neg.	0.1263	Neg.	0.338	Neg.	0.482	Neg.	0	Neg.	0.0538	Neg.	0.0427	Neg.	0.0449	Neg.	0.0259
36437-37-3	Neg.	0.1671	Neg.	0.433	Neg.	0.197	Neg.	0.00185	Neg.	0.154	Neg.	0.0347	Neg.	0.187	Neg.	0.115
3896-11-5	Neg.	0.178	Neg.	0.413	**Pos.**	0.561	Neg.	0.00593	ND		Neg.	0.0331	Neg.	0.229	Neg.	0.14
3846-71-7	Neg.	0.204	Neg.	0.489	Neg.	0.201	Neg.	0.00506	Neg.	0.183	Neg.	0.0351	Neg.	0.225	Neg.	0.137
3864-99-1	Neg.	0.1381	Neg.	0.326	**Pos.**	0.508	Neg.	0.00442	Neg.	0.079	Neg.	0.0391	Neg.	0.226	Neg.	0.134
25973-55-1	Neg.	0.1455	Neg.	0.29	Neg.	0.209	Neg.	0.00138	Neg.	0.127	Neg.	0.0332	Neg.	0.187	Neg.	0.111
70693-49-1	Neg.	0.112	Neg.	0.239	Neg.	0.198	Neg.	0	Neg.	0.0793	Neg.	0.0289	Neg.	0.165	Neg.	0.0942
73936-91-1	Neg.	0.04837	Neg.	0.0821	Neg.	0.204	Neg.	0.126	Neg.	0.404	Neg.	0.0253	Neg.	0.168	Neg.	0.0956
207738-63-4	Neg.	0.0365	Neg.	0.0591	ND		Neg.	0.255	Neg.	0.439	ND		Neg.	0.166	Neg.	0.0907
70321-86-7	Neg.	0.06733	Neg.	0.154	ND		Neg.	0.423	**Pos.**	0.508	Neg.	0.0255	Neg.	0.214	Neg.	0.123
84268-36-0	Neg.	0.1334	Neg.	0.384	ND		ND		ND		ND		Neg.	0.143	Neg.	0.0522
84268-33-7	Neg.	0.1302	Neg.	0.372	ND		ND		ND		ND		Neg.	0.199	Neg.	0.0998
84268-08-6	Neg.	0.08	Neg.	0.344	ND		ND		ND		ND		Neg.	0.154	Neg.	0.0685
84268-23-5	Neg.	0.0616	Neg.	0.304	ND		ND		ND		ND		Neg.	0.0601	Neg.	0.0147
83044-89-7	Neg.	0.0407	Neg.	0.199	ND		ND		ND		ND		Neg.	0.0589	Neg.	0.0142
103597-45-1	Neg.	0.04027	Neg.	0.074	Neg.	0.234	Neg.	0.0698	Neg.	0.286	Neg.	0.0194	Neg.	0.167	Neg.	0.0826
27876-55-7	Neg.	0.135	Neg.	0.274	Neg.	0.211	Neg.	0	Neg.	0.0775	Neg.	0.0512	Neg.	0.177	Neg.	0.102
3147-77-1	Neg.	0.2717	**Pos.**	0.697	**Pos.**	0.972	Neg.	0.00393	Neg.	0.231	Neg.	0.11	Neg.	0.242	Neg.	0.031
2170-39-0	Neg.	0.346	**Pos.**	0.573	**Pos.**	0.515	Neg.	0.0111	ND		Neg.	0.0338	Neg.	0.235	Neg.	0.147

CAS Number	Neurotoxicity					
	pup behavior rodent		pup behavior rat		pup behavior mouse	
	Call	Prob.	Call	Prob.	Call	Prob.
10096-91-0	**Pos.**	0.501	**Pos.**	0.525	ND	
2440-22-4	ND		ND		ND	
3147-76-0	**Pos.**	0.6355	**Pos.**	0.663	ND	
3287-17-0	**Pos.**	0.6155	**Pos.**	0.6395	ND	
3147-75-9	Neg.	0.4105	Neg.	0.4205	ND	
96549-95-0	ND		ND		ND	
83741-30-4	ND		ND		ND	
96478-09-0	ND		ND		ND	
23328-53-2	Neg.	0.191	ND		Neg.	0.00937
36437-37-3	**Pos.**	0.627	**Pos.**	0.6805	ND	
3896-11-5	**Pos.**	0.5125	Neg.	0.429	ND	
3846-71-7	**Pos.**	0.5915	**Pos.**	0.6555	ND	
3864-99-1	**Pos.**	0.56	Neg.	0.446	ND	
25973-55-1	Neg.	0.3655	Neg.	0.408	ND	
70693-49-1	Neg.	0.282	Neg.	0.33	ND	
73936-91-1	Neg.	0.336	ND		Neg.	0.00535
207738-63-4	Neg.	0.381	ND		Neg.	0.498
70321-86-7	Neg.	0.296	ND		Neg.	0
84268-36-0	Neg.	0.422	Neg.	0.4075	Neg.	0.1064
84268-33-7	ND		ND		ND	
84268-08-6	ND		ND		ND	
84268-23-5	ND		ND		ND	
83044-89-7	**Pos.**	0.514	Neg.	0.163	ND	
103597-45-1	Neg.	0.122	ND		Neg.	0
27876-55-7	Neg.	0.3565	Neg.	0.368	ND	
3147-77-1	Neg.	0.2495	Neg.	0.1845	ND	
2170-39-0	ND		ND		ND	

CAS Number	Human Adverse Cardiological Effects											
	electrocardiogram		myocardial		conduction		torsades		arrhythmia		rate rhythm	
	Call	Prob.	Call	Prob.	Call	Prob.	Call	Prob.	Call	Prob.	Call	Prob.
10096-91-0	Neg.	0.1062	Neg.	0.1168	Neg.	0.07852	Neg.	0.08648	Neg.	0.1227	Neg.	0.2385
2440-22-4	Neg.	0.1135	Neg.	0.12	Neg.	0.06424	Neg.	0.1162	Neg.	0.136	Neg.	0.321
3147-76-0	Neg.	0.236	Neg.	0.1638	Neg.	0.07154	Neg.	0.3302	Neg.	0.1503	Neg.	0.2575
3287-17-0	Neg.	0.2383	Neg.	0.1676	Neg.	0.08733	Neg.	0.3428	Neg.	0.1897	Neg.	0.2587
3147-75-9	Neg.	0.1458	Neg.	0.1755	Neg.	0.07292	Neg.	0.1692	Neg.	0.157	Neg.	0.2582
96549-95-0	**Pos.**	0.897	Neg.	0.204	Neg.	0.0533	Neg.	0.0128	Neg.	0.155	Neg.	0.2465
83741-30-4	Neg.	0.158	Neg.	0.22	Neg.	0.08795	Neg.	0.3825	Neg.	0.12	Neg.	0.253
96478-09-0	ND		ND		ND		ND		ND		ND	
23328-53-2	Neg.	0.1388	Neg.	0.07684	Neg.	0.07023	Neg.	0.3535	Neg.	0.1292	Neg.	0.2808
36437-37-3	Neg.	0.241	Neg.	0.1537	Neg.	0.07494	Neg.	0.3796	Neg.	0.143	Neg.	0.2743
3896-11-5	Neg.	0.217	Neg.	0.07884	Neg.	0.08935	Neg.	0.4344	Neg.	0.1753	Neg.	0.3602
3846-71-7	Neg.	0.2397	Neg.	0.1516	Neg.	0.07452	Neg.	0.3723	Neg.	0.1413	Neg.	0.2757
3864-99-1	Neg.	0.2533	Neg.	0.1635	Neg.	0.0661	Neg.	0.3956	Neg.	0.174	Neg.	0.2695
25973-55-1	Neg.	0.158	Neg.	0.1634	Neg.	0.07466	Neg.	0.2377	Neg.	0.1417	Neg.	0.2675
70693-49-1	Neg.	0.1665	Neg.	0.176	Neg.	0.0772	Neg.	0.2574	Neg.	0.1493	Neg.	0.2715
73936-91-1	Neg.	0.389	**Pos.**	0.5243	Neg.	0.06347	Neg.	0.41	Neg.	0.2133	Neg.	0.2705
207738-63-4	Neg.	0.4945	**Pos.**	0.5182	Neg.	0.07853	**Pos.**	0.51	Neg.	0.19	Neg.	0.258
70321-86-7	Neg.	0.3882	**Pos.**	0.5365	Neg.	0.0789	Neg.	0.395	Neg.	0.2107	Neg.	0.272
84268-36-0	Neg.	0.1648	Neg.	0.05542	Neg.	0.03015	Neg.	0.2299	Neg.	0.09183	Neg.	0.1757
84268-33-7	Neg.	0.1527	Neg.	0.0882	Neg.	0.1192	Neg.	0.3727	Neg.	0.1715	Neg.	0.1663
84268-08-6	Neg.	0.178	Neg.	0.0992	Neg.	0.06623	Neg.	0.4093	Neg.	0.2175	Neg.	0.1572
84268-23-5	Neg.	0.1633	Neg.	0.102	Neg.	0.0237	Neg.	0.4173	Neg.	0.229	Neg.	0.1078
83044-89-7	Neg.	0.2807	Neg.	0.1045	Neg.	0.02457	Neg.	0.416	Neg.	0.272	Neg.	0.1665
103597-45-1	Neg.	0.4448	Neg.	0.4788	Neg.	0.06195	Neg.	0.418	Neg.	0.2103	Neg.	0.256
27876-55-7	Neg.	0.1577	Neg.	0.1208	Neg.	0.07252	Neg.	0.1886	Neg.	0.156	Neg.	0.1614
3147-77-1	Neg.	0.1608	Neg.	0.1908	Neg.	0.01761	Neg.	0.2455	Neg.	0.1697	Neg.	0.213
2170-39-0	Neg.	0.1012	Neg.	0.09992	Neg.	0.1754	Neg.	0.2582	Neg.	0.1617	Neg.	0.381

CAS Number	Human Adverse Cardiological Effects													
	palpitations		heart failure		coronary artery		bradycardia		tachycardia		myocardial infarct		QT prolongation	
	Call	Prob.	Call	Prob.	Call	Prob.	Call	Prob.	Call	Prob.	Call	Prob.	Call	Prob.
10096-91-0	Neg.	0.0777	Neg.	0.15	Neg.	0.1693	Neg.	0.1365	Neg.	0.0804	ND		Neg.	0.08656
2440-22-4	Neg.	0.1272	Neg.	0.1787	Neg.	0.213	Neg.	0.1252	Neg.	0.1484	Neg.	0.1736	Neg.	0.09197
3147-76-0	Neg.	0.451	Neg.	0.1727	Neg.	0.2383	Neg.	0.13	Neg.	0.1612	Neg.	0.1753	Neg.	0.1176
3287-17-0	**Pos.**	0.5378	Neg.	0.16	Neg.	0.243	Neg.	0.1112	Neg.	0.1711	Neg.	0.1777	Neg.	0.1538
3147-75-9	Neg.	0.159	Neg.	0.1647	Neg.	0.263	Neg.	0.1257	Neg.	0.1596	Neg.	0.2047	Neg.	0.1374
96549-95-0	Neg.	0.085	Neg.	0.2	Neg.	0.156	Neg.	0.0986	**Pos.**	0.77	Neg.	0.145	Neg.	0.0801
83741-30-4	Neg.	0.189	Neg.	0.245	**Pos.**	0.5575	Neg.	0.1145	Neg.	0.1031	Neg.	0.4168	Neg.	0.08195
96478-09-0	ND		ND		ND		ND		ND		ND		ND	
23328-53-2	Neg.	0.1642	Neg.	0.125	Neg.	0.28	Neg.	0.08058	Neg.	0.1763	Neg.	0.1177	Neg.	0.1426
36437-37-3	Neg.	0.4703	Neg.	0.161	Neg.	0.263	Neg.	0.1297	Neg.	0.192	Neg.	0.09882	Neg.	0.1281
3896-11-5	**Pos.**	0.52	Neg.	0.1557	Neg.	0.2463	Neg.	0.1542	Neg.	0.1883	Neg.	0.1038	Neg.	0.1477
3846-71-7	Neg.	0.467	Neg.	0.1613	Neg.	0.2503	Neg.	0.139	Neg.	0.1919	Neg.	0.09228	Neg.	0.1258
3864-99-1	**Pos.**	0.544	Neg.	0.14	Neg.	0.2497	Neg.	0.1274	Neg.	0.1943	Neg.	0.09995	Neg.	0.162
25973-55-1	Neg.	0.158	Neg.	0.1473	Neg.	0.2633	Neg.	0.1331	Neg.	0.1833	Neg.	0.1005	Neg.	0.1308
70693-49-1	Neg.	0.172	Neg.	0.1373	Neg.	0.284	Neg.	0.1403	Neg.	0.1808	Neg.	0.1116	Neg.	0.1464
73936-91-1	Neg.	0.1768	Neg.	0.1373	Neg.	0.1451	Neg.	0.1489	Neg.	0.1807	Neg.	0.06257	Neg.	0.3014
207738-63-4	Neg.	0.1143	Neg.	0.1395	Neg.	0.1529	Neg.	0.4365	Neg.	0.2605	Neg.	0.0911	Neg.	0.329
70321-86-7	Neg.	0.1745	Neg.	0.1377	Neg.	0.1406	Neg.	0.1588	Neg.	0.1532	Neg.	0.05123	Neg.	0.2984
84268-36-0	Neg.	0.3547	Neg.	0.1475	**Pos.**	0.5467	Neg.	0.03418	Neg.	0.1284	Neg.	0.06823	Neg.	0.06195
84268-33-7	**Pos.**	0.512	Neg.	0.261	**Pos.**	0.5607	Neg.	0.0963	Neg.	0.2317	Neg.	0.4581	Neg.	0.101
84268-08-6	**Pos.**	0.5955	Neg.	0.1985	**Pos.**	0.565	Neg.	0.1092	Neg.	0.1743	Neg.	0.4757	Neg.	0.113
84268-23-5	**Pos.**	0.6085	Neg.	0.1925	**Pos.**	0.5747	Neg.	0.1112	Neg.	0.175	Neg.	0.4827	Neg.	0.1192
83044-89-7	**Pos.**	0.6875	Neg.	0.1425	**Pos.**	0.6385	Neg.	0.1028	Neg.	0.203	Neg.	0.498	Neg.	0.1757
103597-45-1	Neg.	0.1933	Neg.	0.1136	Neg.	0.1754	Neg.	0.1735	Neg.	0.1774	Neg.	0.06576	Neg.	0.3234
27876-55-7	Neg.	0.16	Neg.	0.1477	Neg.	0.2677	Neg.	0.2381	Neg.	0.0857	Neg.	0.1663	Neg.	0.1859
3147-77-1	Neg.	0.1813	Neg.	0.2287	Neg.	0.2343	Neg.	0.1723	Neg.	0.213	Neg.	0.1595	Neg.	0.1463
2170-39-0	Neg.	0.09747	Neg.	0.4043	Neg.	0.2825	Neg.	0.4103	Neg.	0.2792	Neg.	0.09922	Neg.	0.1088

CAS Number	Developmental Toxicity															
	post impl. loss rodent		post impl. loss rat		post impl. loss rabbit		post impl. loss mouse		fetal death rat		fetal death rabbit		fetal death rodent		fetal death mouse	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	Neg.	0.298	Neg.	0.32	Neg.	0.2903	Neg.	0.218	Neg.	0.275	Neg.	0.3245	Neg.	0.2715	Neg.	0.2985
2440-22-4	Neg.	0.29	Neg.	0.32	Neg.	0.3825	Neg.	0.135	Neg.	0.273	Neg.	0.26	Neg.	0.2415	Neg.	0.2265
3147-76-0	Neg.	0.28	Neg.	0.2795	Neg.	0.1911	Neg.	0.197	Neg.	0.2645	Neg.	0.291	Neg.	0.258	Neg.	0.2255
3287-17-0	Neg.	0.254	Neg.	0.262	Neg.	0.1251	Neg.	0.182	Neg.	0.2625	Neg.	0.209	Neg.	0.2525	Neg.	0.2075
3147-75-9	Neg.	0.266	Neg.	0.2725	Neg.	0.2223	Neg.	0.19	Neg.	0.2535	Neg.	0.248	Neg.	0.2435	Neg.	0.216
96549-95-0	Neg.	0.463	Neg.	0.4635	Neg.	0.215	Neg.	0.201	**Pos.**	0.745	Neg.	0.277	**Pos.**	0.5025	Neg.	0.228
83741-30-4	Neg.	0.286	Neg.	0.232	**Pos.**	0.535	Neg.	0.202	Neg.	0.294	Neg.	0.3975	Neg.	0.2695	Neg.	0.294
96478-09-0	Neg.	0.275	Neg.	0.295	ND		ND		Neg.	0.265	ND		Neg.	0.2755	ND	
23328-53-2	Neg.	0.127	Neg.	0.1945	Neg.	0.05069	Neg.	0.0513	Neg.	0.1601	Neg.	0.08115	Neg.	0.1865	Neg.	0.2295
36437-37-3	Neg.	0.204	Neg.	0.2265	Neg.	0.08695	Neg.	0.127	Neg.	0.2535	Neg.	0.144	Neg.	0.243	Neg.	0.2155
3896-11-5	Neg.	0.135	Neg.	0.1925	Neg.	0.00988	Neg.	0.0474	Neg.	0.2605	Neg.	0.0759	Neg.	0.2245	Neg.	0.1905
3846-71-7	Neg.	0.205	Neg.	0.228	Neg.	0.07163	Neg.	0.127	Neg.	0.256	Neg.	0.166	Neg.	0.245	Neg.	0.215
3864-99-1	Neg.	0.178	Neg.	0.2115	Neg.	0.04745	Neg.	0.123	Neg.	0.2625	Neg.	0.111	Neg.	0.2295	Neg.	0.1955
25973-55-1	Neg.	0.192	Neg.	0.2245	Neg.	0.09363	Neg.	0.132	Neg.	0.256	Neg.	0.137	Neg.	0.226	Neg.	0.2085
70693-49-1	Neg.	0.178	Neg.	0.218	Neg.	0.0887	Neg.	0.123	Neg.	0.243	Neg.	0.127	Neg.	0.2075	Neg.	0.194
73936-91-1	Neg.	0.159	Neg.	0.334	Neg.	0.08247	Neg.	0.0945	Neg.	0.2445	Neg.	0.07915	Neg.	0.185	Neg.	0.1465
207738-63-4	Neg.	0.146	Neg.	0.3295	Neg.	0.01485	Neg.	0.095	Neg.	0.2445	Neg.	0.07365	Neg.	0.1665	Neg.	0.1375
70321-86-7	Neg.	0.159	Neg.	0.335	Neg.	0.08163	Neg.	0.0935	Neg.	0.2465	Neg.	0.09215	Neg.	0.1855	Neg.	0.145
84268-36-0	Neg.	0.24	Neg.	0.228	Neg.	0.2903	Neg.	0.124	Neg.	0.1611	Neg.	0.154	Neg.	0.24	Neg.	0.2045
84268-33-7	Neg.	0.253	Neg.	0.21	ND		Neg.	0.15	Neg.	0.255	ND		Neg.	0.277	Neg.	0.213
84268-08-6	Neg.	0.184	Neg.	0.167	ND		Neg.	0.151	Neg.	0.244	ND		Neg.	0.201	Neg.	0.193
84268-23-5	Neg.	0.179	Neg.	0.163	ND		Neg.	0.148	Neg.	0.236	ND		Neg.	0.193	Neg.	0.2315
83044-89-7	Neg.	0.16	Neg.	0.161	Neg.	0.0458	Neg.	0.136	Neg.	0.1426	Neg.	0.0886	Neg.	0.1815	Neg.	0.213
103597-45-1	Neg.	0.145	Neg.	0.322	Neg.	0.0738	Neg.	0.107	Neg.	0.224	Neg.	0.0673	Neg.	0.163	Neg.	0.1545
27876-55-7	Neg.	0.248	Neg.	0.27	Neg.	0.215	Neg.	0.192	Neg.	0.2565	Neg.	0.2355	Neg.	0.2225	Neg.	0.203
3147-77-1	Neg.	0.268	Neg.	0.297	**Pos.**	0.599	Neg.	0.254	Neg.	0.2255	Neg.	0.376	Neg.	0.23	Neg.	0.3455
2170-39-0	Neg.	0.153	Neg.	0.117	ND		Neg.	0.053	**Pos.**	0.615	ND		Neg.	0.271	Neg.	0.213

CAS Number	Developmental Toxicity													
	pre impl. loss rat		pre impl. loss rodent		pre impl. loss rabbit		pre impl. loss mouse		visceral rodent		visceral mouse		visceral rat	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	Neg.	0.2595	Neg.	0.281	Neg.	0.143	Neg.	0.265	Neg.	0.2745	Neg.	0.2327	Neg.	0.2863
2440-22-4	Neg.	0.2985	Neg.	0.232	Neg.	0.1285	Neg.	0.1685	Neg.	0.2775	Neg.	0.2087	Neg.	0.3153
3147-76-0	Neg.	0.301	Neg.	0.274	Neg.	0.1305	Neg.	0.2285	Neg.	0.289	Neg.	0.2283	Neg.	0.302
3287-17-0	Neg.	0.301	Neg.	0.271	Neg.	0.0942	Neg.	0.2145	Neg.	0.2483	Neg.	0.2017	Neg.	0.2803
3147-75-9	Neg.	0.3005	Neg.	0.267	Neg.	0.178	Neg.	0.2195	Neg.	0.2858	Neg.	0.2405	Neg.	0.2867
96549-95-0	**Pos.**	0.709	**Pos.**	0.679	Neg.	0.112	Neg.	0.225	Neg.	0.2563	Neg.	0.187	Neg.	0.331
83741-30-4	Neg.	0.149	Neg.	0.275	Neg.	0.384	Neg.	0.254	Neg.	0.224	Neg.	0.0985	Neg.	0.259
96478-09-0	Neg.	0.281	Neg.	0.2015	ND		ND		Neg.	0.3497	ND		Pos.	0.5033
23328-53-2	Neg.	0.258	Neg.	0.149	Neg.	0.1011	Neg.	0.02849	Neg.	0.4565	Neg.	0.2174	Pos.	0.2853
36437-37-3	Neg.	0.3005	Neg.	0.266	Neg.	0.1148	Neg.	0.219	Neg.	0.2858	Neg.	0.2113	Neg.	0.3083
3896-11-5	Neg.	0.253	Neg.	0.1595	Neg.	0.0305	Neg.	0.08075	Neg.	0.234	Neg.	0.1544	Neg.	0.297
3846-71-7	Neg.	0.3005	Neg.	0.267	Neg.	0.1065	Neg.	0.2195	Neg.	0.2865	Neg.	0.2097	Neg.	0.3107
3864-99-1	Neg.	0.3055	Neg.	0.253	Neg.	0.09197	Neg.	0.2065	Neg.	0.2612	Neg.	0.2123	Neg.	0.3063
25973-55-1	Neg.	0.306	Neg.	0.252	Neg.	0.1375	Neg.	0.216	Neg.	0.2998	Neg.	0.2407	Neg.	0.321
70693-49-1	Neg.	0.3055	Neg.	0.242	Neg.	0.137	Neg.	0.203	Neg.	0.2955	Neg.	0.2523	Neg.	0.2993
73936-91-1	**Pos.**	0.5295	Neg.	0.296	Neg.	0.2103	Neg.	0.1455	Neg.	0.2858	Neg.	0.2015	Neg.	0.4357
207738-63-4	**Pos.**	0.61	Neg.	0.2815	Neg.	0.09605	Neg.	0.1395	Neg.	0.3343	Neg.	0.227	Neg.	0.4413
70321-86-7	**Pos.**	0.529	Neg.	0.2955	Neg.	0.1973	Neg.	0.145	Neg.	0.2855	Neg.	0.198	Neg.	0.4373
84268-36-0	Neg.	0.299	Neg.	0.263	Neg.	0.3873	Neg.	0.22	Neg.	0.2562	Neg.	0.103	Neg.	0.4023
84268-33-7	Neg.	0.259	Neg.	0.297	ND		Neg.	0.246	**Pos.**	0.546	Neg.	0.131	Pos.	0.873
84268-08-6	Neg.	0.321	Neg.	0.265	ND		Neg.	0.181	Neg.	0.308	Neg.	0.162	Pos.	0.693
84268-23-5	Neg.	0.321	Neg.	0.2615	ND		Neg.	0.079	Neg.	0.484	Neg.	0.165	Pos.	0.68
83044-89-7	Neg.	0.318	Neg.	0.2585	Neg.	0.0534	Neg.	0.0767	Neg.	0.324	Neg.	0.154	Pos.	0.681
103597-45-1	**Pos.**	0.5315	Neg.	0.341	Neg.	0.1314	Neg.	0.177	Neg.	0.2973	Neg.	0.2045	Neg.	0.4327
27876-55-7	Neg.	0.3055	Neg.	0.25	Neg.	0.1657	Neg.	0.2115	Neg.	0.3	Neg.	0.1847	Neg.	0.2953
3147-77-1	Neg.	0.285	Neg.	0.2805	Neg.	0.225	Neg.	0.1348	Neg.	0.332	Neg.	0.203	Neg.	0.2413
2170-39-0	Neg.	0.446	Neg.	0.2005	ND		Neg.	0.087	Neg.	0.261	Neg.	0.15	Neg.	0.355

CAS Number	Developmental Toxicity															
	structural mouse		structural rat		structural rodent		structural rabbit		weight dec. rodent		weight dec. mouse		weight dec. rabbit		weight dec. rat	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	Neg.	0.252	Neg.	0.314	Neg.	0.274	Neg.	0.408	Neg.	0.271	Neg.	0.2785	Neg.	0.1825	Neg.	0.2925
2440-22-4	Neg.	0.293	Neg.	0.2905	Neg.	0.28	Neg.	0.462	Neg.	0.212	Neg.	0.2275	Neg.	0.1455	Neg.	0.3155
3147-76-0	Neg.	0.25	Neg.	0.2605	Neg.	0.262	Neg.	0.477	Neg.	0.265	Neg.	0.3085	Neg.	0.1683	Neg.	0.4695
3287-17-0	Neg.	0.249	Neg.	0.2445	Neg.	0.259	Neg.	0.3387	Neg.	0.261	Neg.	0.236	Neg.	0.1325	Neg.	0.466
3147-75-9	Neg.	0.244	Neg.	0.246	Neg.	0.251	Neg.	0.4453	Neg.	0.259	Neg.	0.3085	Neg.	0.1673	Neg.	0.308
96549-95-0	Neg.	0.256	Neg.	0.273	Neg.	0.268	Neg.	0.443	**Pos.**	0.799	Neg.	0.314	Neg.	0.131	**Pos.**	0.8205
83741-30-4	Neg.	0.178	Neg.	0.334	Neg.	0.226	Neg.	0.447	Neg.	0.219	Neg.	0.429	Neg.	0.2845	Neg.	0.2965
96478-09-0	ND		Neg.	0.312	Neg.	0.245	ND		Neg.	0.258	ND		ND		Neg.	0.244
23328-53-2	Neg.	0.36	Neg.	0.195	Neg.	0.23	**Pos.**	0.5227	Neg.	0.193	Neg.	0.2105	Neg.	0.16	Neg.	0.229
36437-37-3	Neg.	0.312	Neg.	0.246	Neg.	0.251	**Pos.**	0.5843	Neg.	0.259	Neg.	0.2985	Neg.	0.1673	Neg.	0.461
3896-11-5	Neg.	0.364	Neg.	0.242	Neg.	0.257	Neg.	0.4707	Neg.	0.204	Neg.	0.1555	Neg.	0.1537	Neg.	0.464
3846-71-7	Neg.	0.313	Neg.	0.2485	Neg.	0.253	**Pos.**	0.601	Neg.	0.258	Neg.	0.297	Neg.	0.1677	Neg.	0.4615
3864-99-1	Neg.	0.326	Neg.	0.2385	Neg.	0.251	Neg.	0.4513	Neg.	0.242	Neg.	0.225	Neg.	0.1483	Neg.	0.4465
25973-55-1	Neg.	0.323	Neg.	0.2455	Neg.	0.248	**Pos.**	0.5677	Neg.	0.244	Neg.	0.297	Neg.	0.161	Neg.	0.293
70693-49-1	Neg.	0.315	Neg.	0.227	Neg.	0.233	**Pos.**	0.5427	Neg.	0.235	Neg.	0.2955	Neg.	0.1603	Neg.	0.281
73936-91-1	Neg.	0.285	Neg.	0.1185	Neg.	0.223	Neg.	0.408	Neg.	0.48	Neg.	0.2255	Neg.	0.1563	**Pos.**	0.5585
207738-63-4	Neg.	0.294	Neg.	0.116	Neg.	0.216	**Pos.**	0.5545	Neg.	0.455	Neg.	0.224	Neg.	0.1377	**Pos.**	0.613
70321-86-7	Neg.	0.286	Neg.	0.12	Neg.	0.224	Neg.	0.423	Neg.	0.478	Neg.	0.225	Neg.	0.1564	**Pos.**	0.56
84268-36-0	Neg.	0.315	Neg.	0.4165	Neg.	0.243	**Pos.**	0.769	Neg.	0.272	Neg.	0.2215	Neg.	0.1947	Neg.	0.4655
84268-33-7	Neg.	0.312	**Pos.**	0.698	Neg.	0.328	ND		Neg.	0.34	Neg.	0.279	ND		Neg.	0.4415
84268-08-6	Neg.	0.315	**Pos.**	0.607	Neg.	0.224	ND		Neg.	0.255	Neg.	0.288	ND		Neg.	0.443
84268-23-5	Neg.	0.311	**Pos.**	0.502	Neg.	0.217	ND		Neg.	0.253	Neg.	0.29	ND		Neg.	0.4385
83044-89-7	Neg.	0.309	Neg.	0.467	Neg.	0.214	Neg.	0.493	Neg.	0.25	Neg.	0.2385	Neg.	0.0823	Neg.	0.4345
103597-45-1	Neg.	0.319	Neg.	0.1185	Neg.	0.211	Neg.	0.4007	**Pos.**	0.507	Neg.	0.2915	Neg.	0.1534	**Pos.**	0.53
27876-55-7	Neg.	0.254	Neg.	0.2425	Neg.	0.246	Neg.	0.427	Neg.	0.24	Neg.	0.304	Neg.	0.1613	Neg.	0.2905
3147-77-1	Neg.	0.189	Neg.	0.3	Neg.	0.221	Neg.	0.4197	Neg.	0.266	Neg.	0.379	Neg.	0.2613	Neg.	0.3015
2170-39-0	Neg.	0.366	Neg.	0.251	Neg.	0.261	ND		Neg.	0.26	Neg.	0.208	ND		**Pos.**	0.532

CAS Number	Developmental Toxicity							
	retardation rodent		retardation rat		retardation mouse		retardation rabbit	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	Neg.	0.238	Neg.	0.292	Neg.	0.2795	Neg.	0.2524
2440-22-4	Neg.	0.245	Neg.	0.3775	Neg.	0.249	Neg.	0.2277
3147-76-0	Neg.	0.268	Neg.	0.3765	Neg.	0.257	Neg.	0.255
3287-17-0	Neg.	0.266	Neg.	0.4135	Neg.	0.255	Neg.	0.1988
3147-75-9	Neg.	0.262	Neg.	0.374	Neg.	0.247	Neg.	0.2706
96549-95-0	Neg.	0.302	Neg.	0.3715	Neg.	0.253	Neg.	0.235
83741-30-4	Neg.	0.231	Neg.	0.2635	Neg.	0.235	Neg.	0.346
96478-09-0	Neg.	0.314	Neg.	0.211	ND		ND	
23328-53-2	Neg.	0.216	Neg.	0.3105	Neg.	0.214	Neg.	0.1495
36437-37-3	Neg.	0.262	Neg.	0.374	Neg.	0.2465	Neg.	0.1542
3896-11-5	Neg.	0.237	Neg.	0.4135	Neg.	0.235	Neg.	0.1413
3846-71-7	Neg.	0.262	Neg.	0.3745	Neg.	0.247	Neg.	0.2049
3864-99-1	Neg.	0.252	Neg.	0.4085	Neg.	0.239	Neg.	0.132
25973-55-1	Neg.	0.25	Neg.	0.369	Neg.	0.236	Neg.	0.1695
70693-49-1	Neg.	0.241	Neg.	0.3665	Neg.	0.222	Neg.	0.1658
73936-91-1	Neg.	0.224	**Pos.**	0.5005	Neg.	0.1415	Neg.	0.133
207738-63-4	Neg.	0.245	**Pos.**	0.5755	Neg.	0.2869	Neg.	0.1177
70321-86-7	Neg.	0.224	**Pos.**	0.501	Neg.	0.1405	Neg.	0.1309
84268-36-0	Neg.	0.256	Neg.	0.417	Neg.	0.2275	Neg.	0.3398
84268-33-7	Neg.	0.256	Neg.	0.3725	Neg.	0.17	ND	
84268-08-6	Neg.	0.244	Neg.	0.3845	Neg.	0.157	ND	
84268-23-5	Neg.	0.241	Neg.	0.3825	Neg.	0.154	ND	
83044-89-7	Neg.	0.238	Neg.	0.4195	Neg.	0.153	**Pos.**	0.5
103597-45-1	Neg.	0.208	Neg.	0.485	Neg.	0.147	Neg.	0.1785
27876-55-7	Neg.	0.249	Neg.	0.3695	Neg.	0.232	Neg.	0.2425
3147-77-1	Neg.	0.227	Neg.	0.277	Neg.	0.2605	Neg.	0.1946
2170-39-0	Neg.	0.294	Neg.	0.492	Neg.	0.24	ND	

CAS Number	Reproductive Toxicity																	
	repro rat male		repro rodent male		repro mouse male		repro rat female		repro mouse female		repro rodent female		sperm rodent		sperm rat		sperm mouse	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	Neg.	0.372	ND		Neg.	0.288	Neg.	0.2607	Neg.	0.247	Neg.	0.3735	Neg.	0.341	Neg.	0.4105	Neg.	0.0982
2440-22-4	Neg.	0.358	Neg.	0.344	ND		Neg.	0.4387	ND		Neg.	0.387	Neg.	0.203	Neg.	0.38	ND	
3147-76-0	Neg.	0.35	Neg.	0.318	ND		Neg.	0.4525	ND		Neg.	0.4198	Neg.	0.295	Neg.	0.3175	ND	
3287-17-0	Neg.	0.187	Neg.	0.233	ND		Neg.	0.4135	Neg.	0.248	Neg.	0.3978	Neg.	0.272	Neg.	0.2095	ND	
3147-75-9	Neg.	0.33	Neg.	0.297	Neg.	0.119	Neg.	0.4703	Neg.	0.244	Neg.	0.418	Neg.	0.282	Neg.	0.259	Neg.	0.0865
96549-95-0	ND		ND		ND		ND		ND		ND		ND		ND		ND	
83741-30-4	ND		ND		ND		**Pos.**	0.792	ND		Neg.	0.24	ND		ND		ND	
96478-09-0	ND		ND		ND		ND		ND		ND		ND		ND		ND	
23328-53-2	Neg.	0.404	Neg.	0.172	Neg.	0.0374	Neg.	0.4817	Neg.	0.107	Neg.	0.1596	Neg.	0.09465	Neg.	0.179	Neg.	0.0493
36437-37-3	**Pos.**	0.715	Neg.	0.296	ND		**Pos.**	0.5098	ND		Neg.	0.3895	Neg.	0.2815	Neg.	0.4305	Neg.	0.0862
3896-11-5	**Pos.**	0.537	Neg.	0.23	ND		Neg.	0.3385	Neg.	0.111	Neg.	0.1943	Neg.	0.09375	Neg.	0.174	ND	
3846-71-7	**Pos.**	0.718	Neg.	0.3	ND		**Pos.**	0.5092	ND		Neg.	0.3943	Neg.	0.284	Neg.	0.468	ND	
3864-99-1	**Pos.**	0.57	Neg.	0.214	Neg.	0.0497	Neg.	0.4335	Neg.	0.114	Neg.	0.3848	Neg.	0.2765	Neg.	0.26	Neg.	0.0293
25973-55-1	**Pos.**	0.745	Neg.	0.281	ND		**Pos.**	0.5355	ND		Neg.	0.4002	Neg.	0.2905	Neg.	0.4545	Neg.	0.0865
70693-49-1	**Pos.**	0.721	Neg.	0.255	ND		**Pos.**	0.5615	ND		Neg.	0.4032	Neg.	0.2735	Neg.	0.3985	Neg.	0.0849
73936-91-1	ND		Neg.	0.233	Neg.	0.0352	**Pos.**	0.5865	Neg.	0.317	Neg.	0.4985	Neg.	0.2695	ND		Neg.	0.052
207738-63-4	ND		Neg.	0.214	Neg.	0.022	Neg.	0.219	Neg.	0.323	Neg.	0.1368	Neg.	0.232	ND		Neg.	0.0507
70321-86-7	ND		Neg.	0.235	Neg.	0.0327	**Pos.**	0.518	Neg.	0.336	**Pos.**	0.502	Neg.	0.2705	ND		Neg.	0.0367
84268-36-0	**Pos.**	0.691	Neg.	0.262	ND		**Pos.**	0.7682	ND		**Pos.**	0.7085	Neg.	0.2825	Neg.	0.4365	ND	
84268-33-7	ND		ND		ND		ND		ND		ND		Neg.	0.26	ND		ND	
84268-08-6	ND		ND		ND		ND		ND		ND		Neg.	0.264	ND		ND	
84268-23-5	ND		ND		ND		ND		ND		ND		Neg.	0.256	ND		ND	
83044-89-7	ND		ND		ND		ND		Neg.	0.00809	Neg.	0.0786	ND		ND		ND	
103597-45-1	ND		Neg.	0.195	Neg.	0.0392	**Pos.**	0.586	Neg.	0.266	**Pos.**	0.5145	Neg.	0.2265	ND		Neg.	0.0812
27876-55-7	Neg.	0.36	Neg.	0.278	ND		**Pos.**	0.5092	ND		Neg.	0.4367	Neg.	0.247	Neg.	0.276	ND	
3147-77-1	Neg.	0.293	Neg.	0.254	Neg.	0.0998	Neg.	0.269	Neg.	0.162	Neg.	0.3262	Neg.	0.2345	Neg.	0.151	Neg.	0.158
2170-39-0	ND		ND		ND		ND		ND		ND		Neg.	0.418	ND		Neg.	0.168

CAS Number	Carcinogenicity											
	BALBc-3T3		C3H10T1-2		cell transformation		SHE		carc mouse		carc mouse female	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	**Pos.**	0.637	ND		**Pos.**	0.641	ND		Neg.	0.339	Neg.	0.3435
2440-22-4	Neg.	0.113	ND		Neg.	0.282	**Pos.**	0.61	Neg.	0.336	Neg.	0.3395
3147-76-0	Neg.	0.268	**Pos.**	0.777	Neg.	0.0374	Neg.	0.034	Neg.	0.3045	Neg.	0.313
3287-17-0	Neg.	0.267	**Pos.**	0.776	Neg.	0.0385	Neg.	0.0214	Neg.	0.2995	Neg.	0.3055
3147-75-9	Neg.	0.188	**Pos.**	0.741	Neg.	0.035	Neg.	0.0747	Neg.	0.277	Neg.	0.281
96549-95-0	Neg.	0.274	ND		Neg.	0.283	**Pos.**	0.657	Neg.	0.3045	Neg.	0.327
83741-30-4	Neg.	0.454	ND		Neg.	0.459	ND		Neg.	0.2735	Neg.	0.3045
96478-09-0	ND		ND		ND		ND		ND		ND	
23328-53-2	Neg.	0.0364	**Pos.**	0.694	Neg.	0.00331	Neg.	0.00309	Neg.	0.224	Neg.	0.1605
36437-37-3	Neg.	0.165	**Pos.**	0.728	Neg.	0.00747	Neg.	0.0122	Neg.	0.2615	Neg.	0.188
3896-11-5	Neg.	0.0746	**Pos.**	0.754	Neg.	0.00486	Neg.	0.00273	Neg.	0.2815	Neg.	0.204
3846-71-7	Neg.	0.23	**Pos.**	0.752	Neg.	0.00701	Neg.	0.00842	Neg.	0.2745	Neg.	0.198
3864-99-1	Neg.	0.254	**Pos.**	0.746	Neg.	0.00808	Neg.	0.00562	Neg.	0.275	Neg.	0.1985
25973-55-1	Neg.	0.182	**Pos.**	0.72	Neg.	0.0105	Neg.	0.0307	Neg.	0.2585	Neg.	0.186
70693-49-1	Neg.	0.172	**Pos.**	0.702	Neg.	0.00757	Neg.	0.0208	Neg.	0.2355	Neg.	0.165
73936-91-1	Neg.	0.177	**Pos.**	0.711	Neg.	0.00788	Neg.	0.00257	Neg.	0.2115	Neg.	0.168
207738-63-4	Neg.	0.0324	**Pos.**	0.638	Neg.	0	Neg.	0.0029	Neg.	0.3005	Neg.	0.407
70321-86-7	Neg.	0.253	**Pos.**	0.745	Neg.	0.0204	Neg.	0.00641	Neg.	0.221	Neg.	0.1775
84268-36-0	Neg.	0.192	**Pos.**	0.706	Neg.	0.00659	Neg.	0.00514	Neg.	0.1935	Neg.	0.122
84268-33-7	Neg.	0.179	**Pos.**	0.641	Neg.	0.00874	Neg.	0.0209	Neg.	0.237	Neg.	0.1745
84268-08-6	Neg.	0.14	**Pos.**	0.664	Neg.	0.00705	Neg.	0.015	Neg.	0.2125	Neg.	0.1235
84268-23-5	Neg.	0.123	**Pos.**	0.629	Neg.	0.00185	Neg.	0.0022	Neg.	0.2015	Neg.	0.116
83044-89-7	Neg.	0.122	**Pos.**	0.628	Neg.	0.00191	Neg.	0.00137	Neg.	0.1975	Neg.	0.112
103597-45-1	Neg.	0.222	**Pos.**	0.679	Neg.	0.0304	Neg.	0.0267	Neg.	0.197	Neg.	0.139
27876-55-7	Neg.	0.209	**Pos.**	0.732	Neg.	0.0339	Neg.	0.0843	Neg.	0.2365	Neg.	0.254
3147-77-1	**Pos.**	0.551	**Pos.**	0.679	Neg.	0.0159	Neg.	0.0438	Neg.	0.25	Neg.	0.2245
2170-39-0	Neg.	0.075	**Pos.**	0.756	Neg.	0.0255	Neg.	0.176	Neg.	0.2865	Neg.	0.212

CAS Number	Carcinogenicity									
	carc mouse male		carc rat		carc rat female		carc rat male		carc rodent	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	ND		Neg.	0.423	ND		ND		Neg.	0.3635
2440-22-4	ND		Neg.	0.422	ND		ND		Neg.	0.362
3147-76-0	Neg.	0.2935	Neg.	0.352	Neg.	0.2795	Neg.	0.354	Neg.	0.3245
3287-17-0	Neg.	0.288	Neg.	0.284	Neg.	0.2315	Neg.	0.246	Neg.	0.322
3147-75-9	Neg.	0.269	Neg.	0.3165	Neg.	0.252	Neg.	0.3165	Neg.	0.2805
96549-95-0	Neg.	0.2965	Neg.	0.381	Neg.	0.2695	Neg.	0.3475	Neg.	0.3325
83741-30-4	Neg.	0.212	Neg.	0.3125	Neg.	0.26	Neg.	0.277	Neg.	0.304
96478-09-0	ND		ND		ND		ND		ND	
23328-53-2	Neg.	0.3545	Neg.	0.248	Neg.	0.238	Neg.	0.2995	Neg.	0.221
36437-37-3	Neg.	0.269	Neg.	0.2605	Neg.	0.252	Neg.	0.3095	Neg.	0.28
3896-11-5	Neg.	0.403	Neg.	0.2325	Neg.	0.2315	Neg.	0.2425	Neg.	0.3105
3846-71-7	Neg.	0.2775	Neg.	0.2905	Neg.	0.279	Neg.	0.345	Neg.	0.307
3864-99-1	Neg.	0.2855	Neg.	0.233	Neg.	0.2335	Neg.	0.245	Neg.	0.3015
25973-55-1	Neg.	0.2725	Neg.	0.261	Neg.	0.2535	Neg.	0.3125	Neg.	0.264
70693-49-1	Neg.	0.248	Neg.	0.2575	Neg.	0.2515	Neg.	0.3085	Neg.	0.253
73936-91-1	Neg.	0.251	Neg.	0.2565	Neg.	0.382	Neg.	0.4105	Neg.	0.238
207738-63-4	Neg.	0.249	Neg.	0.2575	Neg.	0.365	Neg.	0.414	Neg.	0.2295
70321-86-7	Neg.	0.259	Neg.	0.286	Neg.	0.4155	Neg.	0.448	Neg.	0.27
84268-36-0	Neg.	0.2315	Neg.	0.1353	Neg.	0.152	Neg.	0.1515	Neg.	0.186
84268-33-7	Neg.	0.2525	Neg.	0.2375	Neg.	0.237	Neg.	0.28	Neg.	0.262
84268-08-6	Neg.	0.196	Neg.	0.226	Neg.	0.2325	Neg.	0.3145	Neg.	0.2285
84268-23-5	Neg.	0.186	Neg.	0.223	Neg.	0.229	Neg.	0.3095	Neg.	0.203
83044-89-7	Neg.	0.182	Neg.	0.1735	Neg.	0.187	Neg.	0.212	Neg.	0.201
103597-45-1	Neg.	0.207	Neg.	0.245	Neg.	0.3705	Neg.	0.399	Neg.	0.227
27876-55-7	Neg.	0.2705	Neg.	0.3195	Neg.	0.2565	Neg.	0.322	Neg.	0.2725
3147-77-1	Neg.	0.233	Neg.	0.2845	Neg.	0.2215	Neg.	0.3315	Neg.	0.1925
2170-39-0	Neg.	0.4115	Neg.	0.29	Neg.	0.2765	Neg.	0.277	Neg.	0.3215

CAS Number	Human Adverse Hepatobiliary Effects									
	enzyme release		bile duct		jaundice		liver acute		gall bladder	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	ND		Neg.	0.09	ND		ND		ND	
2440-22-4	Neg.	0.143	Neg.	0.09025	ND		Neg.	0.0914	Neg.	0.165
3147-76-0	Neg.	0.122	Neg.	0.0911	Neg.	0.1857	Neg.	0.1022	Neg.	0.151
3287-17-0	Neg.	0.148	Neg.	0.0915	Neg.	0.1893	Neg.	0.1433	Neg.	0.152
3147-75-9	Neg.	0.08547	Neg.	0.09005	Neg.	0.1197	Neg.	0.0965	Neg.	0.154
96549-95-0	Neg.	0.163	Neg.	0.0913	ND		Neg.	0.0851	Neg.	0.139
83741-30-4	Neg.	0.165	Neg.	0.1179	Neg.	0.4535	Neg.	0.2713	Neg.	0.3805
96478-09-0	ND		ND		ND		ND		ND	
23328-53-2	Neg.	0.09177	Neg.	0.0989	Neg.	0.1883	Neg.	0.122	Neg.	0.2
36437-37-3	Neg.	0.08547	Neg.	0.0939	Neg.	0.12	Neg.	0.1275	Neg.	0.1725
3896-11-5	Neg.	0.1717	Neg.	0.09595	Neg.	0.191	Neg.	0.171	Neg.	0.19
3846-71-7	Neg.	0.119	Neg.	0.09615	Neg.	0.192	Neg.	0.1295	Neg.	0.172
3864-99-1	Neg.	0.145	Neg.	0.0964	Neg.	0.1847	Neg.	0.151	Neg.	0.1715
25973-55-1	Neg.	0.08447	Neg.	0.09445	Neg.	0.1146	Neg.	0.1139	Neg.	0.1735
70693-49-1	Neg.	0.08063	Neg.	0.09625	Neg.	0.1206	Neg.	0.1069	Neg.	0.1775
73936-91-1	Neg.	0.08167	Neg.	0.0963	Neg.	0.1063	Neg.	0.1077	Neg.	0.177
207738-63-4	Neg.	0.156	Neg.	0.102	Neg.	0.239	Neg.	0.1314	Neg.	0.172
70321-86-7	Neg.	0.111	Neg.	0.1069	Neg.	0.182	Neg.	0.1086	Neg.	0.176
84268-36-0	Neg.	0.1207	Neg.	0.0935	Neg.	0.1857	Neg.	0.1212	Neg.	0.219
84268-33-7	Neg.	0.054	ND		Neg.	0.137	Neg.	0.14	ND	
84268-08-6	Neg.	0.0489	ND		Neg.	0.128	Neg.	0.12	ND	
84268-23-5	Neg.	0.0474	ND		Neg.	0.126	Neg.	0.116	ND	
83044-89-7	Neg.	0.06225	ND		Neg.	0.1495	Neg.	0.1323	ND	
103597-45-1	Neg.	0.07903	Neg.	0.1026	Neg.	0.129	Neg.	0.0802	Neg.	0.1935
27876-55-7	Neg.	0.09517	Neg.	0.09085	Neg.	0.1173	Neg.	0.0856	Neg.	0.1545
3147-77-1	Neg.	0.226	Neg.	0.101	Neg.	0.1975	Neg.	0.1194	ND	
2170-39-0	Neg.	0.138	Neg.	0.0999	ND		Neg.	0.151	Neg.	0.167

CAS Number	Human Adverse Urinary Effects											
	kidney function		kidney		urolithiasis		nephropathy		bladder		blood urine	
	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability	Call	Probability
10096-91-0	ND		ND		ND		ND		Neg.	0.1737	ND	
2440-22-4	ND		ND		ND		ND		Neg.	0.1633	ND	
3147-76-0	Neg.	0.1463	ND		Neg.	0.139	ND		Neg.	0.164	ND	
3287-17-0	Neg.	0.1453	ND		Neg.	0.1455	ND		Neg.	0.1967	ND	
3147-75-9	Neg.	0.144	ND		Neg.	0.1245	ND		Neg.	0.1383	ND	
96549-95-0	ND		ND		Neg.	0.129	ND		Neg.	0.136	ND	
83741-30-4	Neg.	0.1623	ND		Neg.	0.131	Neg.	0.1865	Neg.	0.1497	Neg.	0.18
96478-09-0	ND		ND		ND		ND		ND		ND	
23328-53-2	ND		Neg.	0.0803	ND		ND		Neg.	0.1833	Neg.	0.0655
36437-37-3	Neg.	0.144	ND		Neg.	0.1245	ND		Neg.	0.1737	ND	
3896-11-5	Neg.	0.1453	ND		Neg.	0.1455	ND		Neg.	0.1983	ND	
3846-71-7	Neg.	0.1443	ND		Neg.	0.1385	ND		Neg.	0.172	ND	
3864-99-1	Neg.	0.1483	ND		Neg.	0.1445	ND		Neg.	0.189	ND	
25973-55-1	Neg.	0.148	ND		Neg.	0.124	ND		Neg.	0.163	ND	
70693-49-1	Neg.	0.145	ND		Neg.	0.1235	ND		Neg.	0.14	ND	
73936-91-1	Neg.	0.09963	ND		Neg.	0.092	Neg.	0.139	Neg.	0.173	ND	
207738-63-4	Neg.	0.103	ND		Neg.	0.0916	Neg.	0.124	Neg.	0.166	ND	
70321-86-7	Neg.	0.1009	ND		Neg.	0.1024	Neg.	0.14	Neg.	0.2103	ND	
84268-36-0	Neg.	0.2485	Neg.	0.167	Neg.	0.145	Neg.	0.2187	Neg.	0.1647	Neg.	0.2687
84268-33-7	Neg.	0.15	Neg.	0.133	ND		Neg.	0.13	Neg.	0.132	Neg.	0.11
84268-08-6	Neg.	0.154	Neg.	0.156	Neg.	0.124	Neg.	0.0969	Neg.	0.125	Neg.	0.069
84268-23-5	Neg.	0.153	Neg.	0.156	Neg.	0.124	Neg.	0.0936	Neg.	0.128	Neg.	0.0515
83044-89-7	Neg.	0.1757	Neg.	0.1405	Neg.	0.1323	Neg.	0.1284	Neg.	0.195	Neg.	0.0552
103597-45-1	Neg.	0.1195	ND		Neg.	0.09615	Neg.	0.162	Neg.	0.1757	ND	
27876-55-7	Neg.	0.1477	ND		Neg.	0.124	ND		Neg.	0.1317	ND	
3147-77-1	ND		Neg.	0.0839	Neg.	0.1433	Neg.	0.17	Neg.	0.1508	Neg.	0.2748
2170-39-0	Neg.	0.4005	ND		Neg.	0.219	ND		Neg.	0.1526	Neg.	0.3325

Abbreviations: ND = Not in Domain, Neg. = Negative, Pos. = Positive